CUMULATIVE EXPOSURE TOXICITY DATABASE

USER'S MANUAL

Prepared for:

Office of Policy U.S. Environmental Protection Agency

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INTRODUCTION CHAPTER 1

EPA's Office of Policy is conducting a Cumulative Exposure Study to assess exposure to multiple pollutants across multiple exposure pathways. The goal of the project is to increase understanding of cumulative exposure to contaminants in the environment. EPA anticipates that this project will allow the Agency to:

- 1. Estimate the average levels of cumulative exposure to different demographic subpopulations across the U.S., and
- 2. Identify subpopulations with exposure levels that differ significantly from the average U.S. exposure and determine the basis for such differences.

The study is also an important step in developing strategies to better target national and state environmental policies and regulations at protecting populations experiencing the greatest exposures.

The Cumulative Exposure Study is assessing national exposure levels for three exposure pathways: inhalation of pollutants in air, ingestion of contaminants in food, and ingestion of pollutants in drinking water. EPA is evaluating exposures from each pathway in separate analyses, and considering methodological options for comparing these three components to provide useful information regarding cumulative multipathway exposures.

Toxicological information is key to understanding the potential public health impacts associated with the national estimates of toxics concentrations in air, food, and drinking water developed under the Cumulative Exposure Study. EPA and other agencies such as the Agency for Toxic Substances and Disease Registry (ATSDR) and the California EPA (CAL EPA), have collected large amounts of data on the toxicological effects of many pollutants by various exposure pathways. These agencies have developed health benchmark values for these pollutants based on the toxicological data collected. While useful, these benchmarks are narrow in focus and are often based on toxicity data for only one of the potentially many health effects associated with a particular pollutant. Furthermore, benchmarks may vary from agency to agency not only in value but in the health effect considered as well.

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In order to obtain a more comprehensive picture of the potential public health impacts associated with the estimated cumulative exposure levels, EPA has developed the Cumulative Exposure Toxicity Database (the database). The database is an extensive compilation of toxicological data obtained from multiple sources both within and outside of EPA and contains both quantitative data, including peer-reviewed benchmark values and values derived from primary literature, and qualitative information on health effects. To help the user sort through this vast amount of information, the database contains a user interface designed to provide quick and easy access to desired toxicological information.

It is important to note that the base of toxicological knowledge is not static; it is continually changing and expanding. Regulatory benchmarks for previously tested compounds are being re-evaluated in light of new data, and studies are being conducted to obtain toxicity data for as yet untested chemicals. Thus, the Cumulative Exposure Toxicity Database consists of a snapshot of toxicological data as of a specified "freeze date" -- December 1997, for this version -- and may not reflect changes that have occurred since that time.

Although initially developed for use with the Cumulative Exposure Study, the database is likely to have wider reaching applications as well. The extensive list of chemicals included, the presence of multiple sources of data, and the easy-to-use interface make the Cumulative Exposure Toxicity Database a valuable tool for anyone conducting a human health risk assessment or other analysis requiring toxicological data.

HOW TO USE THIS MANUAL

This manual provides instructions for using the Cumulative Exposure Toxicity Database, a Microsoft AccessTM database that includes a user interface featuring pre-programmed search functions. The database is available in two versions:

- 1. An .mdb file that can only be opened using Microsoft AccessTM 7.0. In addition to the pre-programmed functions, this version (the AccessTM 7.0 version) allows users to view the underlying data tables and design their own queries.
- 2. A self-contained executable program that uses Microsoft Access Run-TimeTM to enable users to operate the database even if AccessTM is not present. This version (the Run-TimeTM version) only allows users to run the pre-programmed searches of the user interface and does not allow them to view the underlying data tables.

Users without AccessTM must use the Run-TimeTM version. Users with AccessTM can use either version. We recommend using the AccessTM 7.0 version because of its increased functionality; however, users less comfortable with AccessTM or with databases in general may prefer to use the Run-TimeTM version. Information on choosing a version is presented in the *Getting Started* section of Chapter 2.

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This manual is divided into two major sections. Chapter 2 presents an overview of the database that introduces the user to its structure and function and helps the user get started. This chapter also includes examples that illustrate the operation of the searches that are built into the user interface. With the exception of the *Beyond the Interface* section, which contains information specific to the AccessTM 7.0 version, this chapter contains information useful to users of both versions of the database.

Chapter 3 presents more detailed technical information concerning the design and structure of the database and the data sources used to develop it. This section is primarily designed to be a technical reference for the more advanced user who is familiar with databases in general and with Microsoft AccessTM in particular. Thus, Chapter 3 is likely to be most useful to users of the Access 7.0 version, whose interaction with the database will not be limited solely to the user interface. However, this section could also be useful for users who wish to obtain more information about the data sources that provided information for the database.

Much of the key information presented in this manual is also included in on-line help screens in the database program itself. The screens that appear in the database should be self-explanatory. If they are not, we have included a Help button. Clicking this button will bring up one or more help screens that provide clarification.

Please note that this manual assumes a certain basic level of familiarity and comfort with the WindowsTM 95 operating environment. If you are not familiar with Windows 95TM, please consult a Microsoft WindowsTM 95 user's guide. Although the user interface enables you to use the database even if you are unfamiliar with Microsoft AccessTM, you may wish to increase your comfort level with the database by consulting an AccessTM user's guide.

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The Cumulative Exposure Toxicity Database is an interactive database of toxicological data designed for IBM-PC compatible computers. This chapter focuses on familiarizing the user with the structure and function of the database and presents basic instructions for its use. For an in-depth discussion of more technical aspects of the database please consult Chapter 3.

This chapter is divided into two sections. The first presents an overview of the database program and its functions. The second provides detailed instructions for operating the database, examples illustrating various uses of the database, and troubleshooting suggestions.

DATABASE OVERVIEW

The Cumulative Exposure Toxicity Database combines a comprehensive database of toxicological information from multiple respected data sources with an easy-to-use interface that allows retrieval of data according to user-specified criteria. The database itself comprises several tables of data. Exhibit 2-1 provides an overview of the main tables of the database and the types of data in each. As a reminder, users of the Run-TimeTM version cannot access these tables directly.

The user interface allows the user to find specific data of interest. For example, using the pre-programmed searches, the user could:

- Obtain cancer toxicity benchmarks for oral exposures to all pollutants analyzed in the food portion of the Cumulative Exposure Study;
- Retrieve specific toxicity data for an individual chemical or a user-defined group of chemicals;
- Retrieve Lowest Observed Adverse Effect Levels (LOAELs) and No Observed Adverse Effect Levels (NOAELs) for all compounds in the database containing mercury; or
- Obtain toxicity values for all chemicals in the database exhibiting neurotoxic effects.

Exhibit 2-1				
OVERVIEW OF TABLES	OVERVIEW OF TABLES IN CUMULATIVE EXPOSURE TOXICITY DATABASE			
Table Name Description				
General Information Table	Basic information about each chemical analyzed.			
Cancer Health Effects Table	Cancer toxicity data for both oral and inhalation exposures.			
Non-cancer Health Effects Table	Benchmark values for acute, subchronic, and chronic non-cancer health effects for both oral and inhalation exposures.			
Qualitative Health Effects Table	Qualitative health effect information from EPA's <i>Health Effects</i> Notebook for Hazardous Air Pollutants. ¹			
Oral NOAEL/LOAEL Table	No Observed Adverse Effect Levels, Lowest Observed Adverse Effect Levels, and LD ₅₀ s for non-cancer health effects related to oral exposures. ²			
Inhalation NOAEL/LOAEL Table	No Observed Adverse Effect Levels, Lowest Observed Adverse Effect Levels, and LC ₅₀ s, for non-cancer health effects related to inhalation exposures. ²			
PAH Toxic Equivalency Factor Table	Toxic Equivalency Factors (TEFs) published by EPA for relating the carcinogenic potency of certain polycyclic aromatic hydrocarbons (PAHs) to that of benzo[a]pyrene (BaP). ³			
Chemical Synonym Table	Synonyms for chemicals in the database.			
Data Sources	List of the sources of the toxicological information in the database.			

¹ U.S. Environmental Protection Agency, *Health Effects Notebook for Hazardous Air Pollutants*, March 1995.

While the interface facilitates data retrieval for both novice and expert users alike, it is not intended to discourage experienced users of AccessTM 7.0 from designing their own queries and taking advantage of the fully functional database underlying the interface. These options are not available for users of the Run-TimeTM version of the database, however.

The database contains data for 344 chemicals or groups of chemicals. The chemicals included in the database are listed alphabetically in Appendix A. Approximately half of these are chemicals analyzed in the air, water, and/or food portions of EPA's Cumulative Exposure Study. The remainder of the compounds, while not specifically evaluated in this study, are members of a chemical group that was evaluated (e.g., Aroclor 1260 was not specifically analyzed, but PCBs were.) Twenty-one such chemical groups are present in the database. Appendix B presents a list of the groups and the chemicals in the database which belong to each group.

Several data sources were used to construct the database. In selecting sources, we focused on widely used data sets that contain toxicological benchmarks and potency measures, as well as qualitative toxicity information. The following sources provided data for the database:

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² See Appendix C for a glossary of acronyms used in the database.

³ U.S. Environmental Protection Agency, *Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons*, EPA/600/R-93/089, July 1993.

- Agency for Toxic Substances and Disease Registry, Minimal Risk Levels
 for Hazardous Substances, December 1997, obtained from
 http://www.atsdr1.atsdr.cde.gov:8080/hrls.html, March 1998;
- Agency for Toxic Substances and Disease Registry, *Toxicological Profiles* on CD-ROM, CRC Press, Inc., 1997;
- California Air Pollution Control Officers' Association, *Air Toxics "Hot Spots" Program Risk Assessment Guidelines*, October, 1993.
- California Environmental Protection Agency, Risk Assessment Advisory Committee, A Review of the California Environmental Protection Agency's Risk Assessment Practices, Policies, and Guidelines, 1996;
- California Environmental Protection Agency, Standards and Criteria Work Group, California Potency Factors: Update, April 1, 1996, obtained from http://www.calepa.cahwnet.gov/oehha/docs/covrltrb.htm;
- International Agency for Research on Cancer (IARC), weights of evidence (WOE) for Carcinogenicity in Humans, February 28, 1997, obtained from http://www.iarc.fr/monoeval/grlist.htm, November 21, 1997;
- U.S. Environmental Protection Agency, *Technical Background Document to Support Rulemaking Pursuant to the Clean Air Act Section 112(g): Ranking of Pollutants with Respect to Hazard to Human Health*, EPA-450/3-92-010, February 1994;
- U.S. Environmental Protection Agency, Documentation of De Minimis Emission Rates Proposed 40 CFR Part 63, Subpart B Background Document, EPA-453/R-93-035, February 1994;
- U.S. Environmental Protection Agency, *Hazardous Air Pollutants: Profiles of Non-cancer Toxicity from Inhalation Exposures* (HAPs Profiles), September 1993;
- U.S. Environmental Protection Agency, *Health Effects Notebook for Hazardous Air Pollutants* (HAPfacts), December 1994;
- U.S. Environmental Protection Agency, *Health Effects Assessment Summary Tables* (HEAST), in Pioneer Systems Development, *Smarttox Toxicity Value Lookup Tables*, December 1997;
- U.S. Environmental Protection Agency, *The Integrated Risk Information System* (IRIS) in Pioneer Systems Development, *Smarttox Toxicity Value Lookup Table*, December 1997;

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- U.S. Environmental Protection Agency, *Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons*, EPA/600/R-93/089, July 1993.
- U.S. Environmental Protection Agency, *Technical Guidance for Hazards Analysis*, *Emergency Planning for Extremely Hazardous Substances*, December 1987 (SARA Title III); and
- U.S. National Library of Medicine, Hazardous Substances Data Bank (HSDB), accessed December 1997 and April 1998.

We selected the data sources listed above based on the applicability of the toxicological information to the needs of the Cumulative Exposure Study, the number of chemicals for which there is available information, and the reliability and age of the data. Each source represents the most current version available as of December 1997; however, some sources (e.g., HAPs Profiles, September 1993) are older than others (e.g., IRIS, December 1997). The user should consider the relative age of the sources when using data obtained from the Cumulative Exposure Toxicity Database.

USING THE DATABASE

This section describes how to install and use the database. The *Getting Started* section discusses hardware requirements and installing the database. The *User Interface* section describes the built-in database searches and how to use them. For AccessTM 7.0 users, the *Beyond the Interface* section briefly describes how to bypass the interface and work with the data tables directly. Finally, the *Troubleshooting* section presents some common problems and their solutions.

Getting Started

The Cumulative Exposure Toxicity Database requires the following *minimum* hardware and software to operate:

- IBM-PC compatible 486 computer (66 MHz)
- 16 MB of RAM
- WindowsTM 95 operating system
- Microsoft AccessTM (version 7.0) for Windows 95 (optional)
- Monitor with 640 x 480 or greater resolution
- 10 MB free hard drive space for AccessTM 7.0 users (20 MB for Run-TimeTM users)
- Mouse (or other pointing device)

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The *recommended* configuration for running the database is:

- IBM-PC compatible Pentium computer (90 MHz or faster)
- At least 24 MB of RAM
- WindowsTM 95 operating system
- Microsoft AccessTM (version 7.0) for Windows 95 (optional)
- SVGA Monitor running at 800 x 600 resolution or greater¹
- 20 MB free hard drive space for AccessTM 7.0 users (30 MB for Run-TimeTM users)
- Mouse (or other pointing device)

The database is originally compressed as a .ZIP file named CEDBMMYY.ZIP, where MM and YY are the release month and year, respectively of the database. After decompressing the database, select Run from the Start menu in Windows 95, type "path\ SETUP.EXE" (where path\ is the directory where the setup file is located), and click OK. The setup program will first request that all other applications be closed and then will ask the user to specify a location to install the database (C:\CETDB is the default). Next, the user must choose one of three setup options:

- **Standard.** This option installs the Run-Time[™] version of the database (the database file plus all the Run Time Access[™] components). Users without Access[™] 7.0 should use this option.
- **Compact.** This option installs only the database .mdb file (the AccessTM 7.0 version). Users without AccessTM 7.0 should not choose this option.
- **Custom.** This option allows the user to specify the files installed.

After the setup has successfully installed the appropriate files, open the database by selecting *Programs: Cumulative Exposure Toxicity Database* from the *Start* menu.

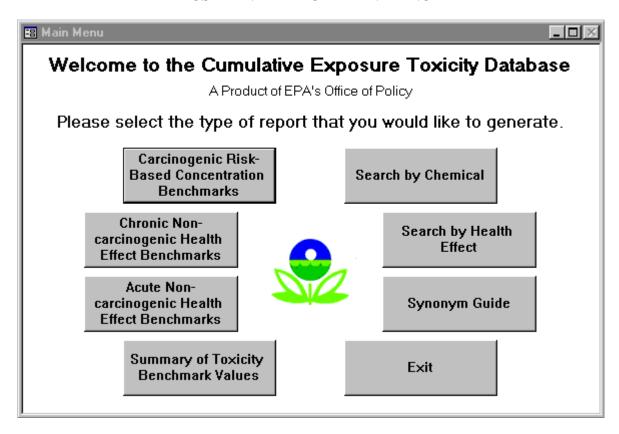
The User Interface

Upon opening the database, the program displays the Main Menu of the user interface, which is shown in Exhibit 2-2.

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¹ The database interface screens were designed at a resolution of 800 x 600. For the best appearance, it is highly recommended that the database be used with a monitor resolution of 800 x 600. Screen resolution can be changed by selecting *Settings: Control Panels* from the *Start* menu, double clicking on *Display*, and selecting the *Settings* tab. For further information, the user should consult a guide to Windows[™] 95 or the user's guide for the monitor.

Exhibit 2-2
USER INTERFACE MAIN MENU



The interface is designed to make the database more user-friendly and to improve data accessibility for those unfamiliar with Microsoft AccessTM. The interface automates several basic searches for toxicological data, while providing users with sufficient flexibility to tailor these searches to meet their needs. The main interface screen allows the user to choose from among the following seven pre-defined searches:

- Carcinogenic Risk-Based Concentration Benchmarks
- Chronic Non-carcinogenic Health Effect Benchmarks
- Acute Non-carcinogenic Health Effect Benchmarks
- Summary of Toxicity Benchmark Values
- Search by Chemical
- Search by Health Effect
- Synonym Guide

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The interface presents a window with seven buttons corresponding to the seven searches plus a *Close* button that exits the interface.² To execute a search, simply click on the desired button and follow the directions presented. Some searches involve several screens of input. The *Back* buttons present in most of the windows allow the user to move back to previous screens to review or change selected options before executing the search. We describe the seven search options in detail below.

The "Benchmark" Searches

The four buttons on the left side of the main menu execute similar data searches. They generate tables of "benchmark concentrations" -- concentrations representing potential regulatory thresholds of concern for human health. These benchmark values are based on currently available toxicity measures (e.g., unit risks, reference concentrations) and can be compared with national exposure levels from the Cumulative Exposure Study or other exposure or concentration data.

In order to make the database as comprehensive as possible, toxicity data from several sources have been included in the database. Some chemicals may have toxicity data from only one source, while others may have data reported in several sources. Because the different sources vary in their methodology for developing toxicity values, their selection of data, their characterization of uncertainty, and their level of peer review, we have developed a mechanism for selecting the most appropriate toxicity value on which to base benchmark concentrations. The benchmark searches operate according to pre-set hierarchies of data sources. In these hierarchies, Tier I consists of EPA-derived values with the lowest uncertainties, consistency in derivation, and the most comprehensive peer review. The lower tiers consist of values with increasing levels of uncertainty, less methodological consistency, and less peer review.

Based on the user's search criteria, the database identifies the highest tier toxicity value available for each compound according to the applicable hierarchy of data types and sources and reports the associated benchmark. Because a data hierarchy is used, these tables do not contain all benchmarks in the database for a given chemical. To obtain all the toxicity data on a particular chemical, use the Search by Chemical Search.

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 $^{^2}$ In order to by-pass the interface and explore the database directly, simply click on the Close button.

³ The data hierarchies developed specifically for the "benchmark" queries are based upon data hierarchies developed in Caldwell, Jane C., Tracey J. Woodruff, Rachel Morello-Frosch, and Daniel A. Axelrad, "Application of Health Information to Hazardous Air Pollutants Modeled in EPA's Cumulative Exposure Project," *Toxicology and Industrial Health*, vol. 14, p. 429-54, 1998. This paper can also be downloaded from http://www.epa.gov/oppecumm/CEPpapers/paper CWMA.pdf.

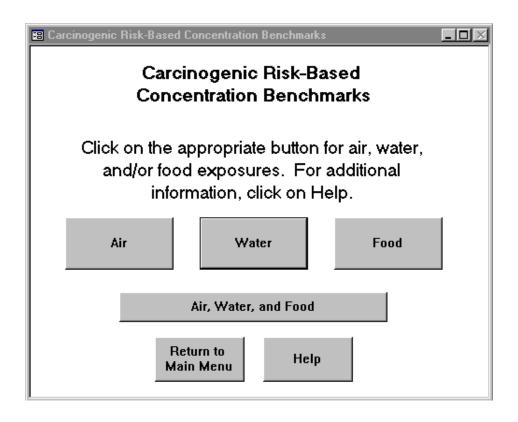
The four benchmark searches in the database are: Carcinogenic Risk-Based Concentration Benchmarks, Acute Non-carcinogenic Health Effect Benchmarks, Chronic Non-carcinogenic Health Effects Benchmarks, and Summary of Toxicity Benchmark Values. The first three searches provide toxicity data for a particular type of toxicity (cancer, non-cancer) or a specific exposure duration (chronic, acute), and each uses a different hierarchy, as discussed below. The Summary Search essentially combines the first three searches into one and creates a summary table of cancer and non-cancer benchmarks based on the appropriate hierarchies. This summary table, however, provides less detail about the benchmark values than the individual searches.

When running any of the benchmark searches the user must select the set of chemicals on which to conduct the search. The program provides the following two options:

- Cumulative Exposure Study Chemicals. If the user selects the *Cumulative Exposure Study* option, the database will ask the user to specify a medium (see Exhibit 2-3) and will limit the search to those chemicals analyzed in the specified component of the Cumulative Exposure Study (i.e., air, water, food). Because this option limits the data presented, it is recommended only for use with data from the Cumulative Exposure Study. The *All Chemicals* option is more appropriate for general use.
- All Chemicals. If the user chooses the *All Chemicals* option, the query will ask the user to specify an exposure route (see Exhibit 2-4) and will search through available data for all of the chemicals in the database, regardless of whether those compounds were evaluated in the corresponding component of the Cumulative Exposure Study.

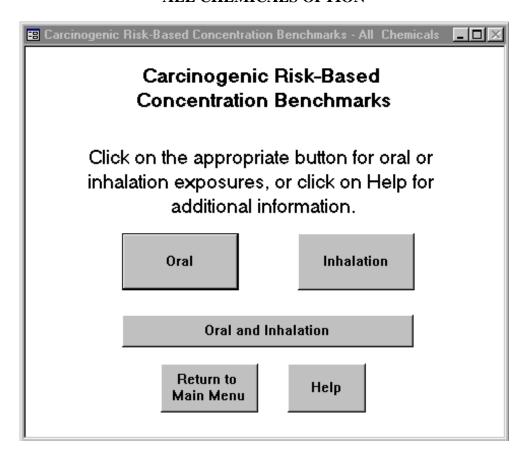
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Exhibit 2-3
CUMULATIVE EXPOSURE STUDY OPTION



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Exhibit 2-4
ALL CHEMICALS OPTION



The following sections describe the individual "benchmark" queries in greater detail.

Carcinogenic Risk-Based Concentration Benchmarks

This query creates a table of chemical concentration benchmarks that correspond to a one in one million excess lifetime cancer risk. The risk-based concentrations are calculated by dividing $1x10^{-6}$ by the best available carcinogenic potency value (unit risk for inhalation, cancer slope factor for oral) for each compound. The best available value is determined by the data hierarchy presented in Exhibit 2-5. The query searches for the highest tier potency value for each compound in each medium and presents that value and the risk-based concentration derived from that value. If a compound has a Weight of Evidence (WOE) classification from either EPA or IARC but no quantitative toxicity values, that compound is included in the query output with its Weight of Evidence, but no risk-based concentration is calculated.

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Exhibit 2-5				
D	DATA HIERARCHY FOR CARCINOGENIC RISK-BASED CONCENTRATION BENCHMARKS Exposure Route			
Tier	Priority	Inhalation	Oral	
Ia	1	IRIS inhalation unit risk (UR)	IRIS oral cancer slope factor (CSF)	
Ib	2	112 (DOC) UR	112(DOC) CSF	
IIa	3	IRIS oral CSF converted into inhalation UR ⁴	CAL EPA oral CSF	
IIb	4	CAL EPA inhalation UR	HEAST oral CSF	
IIc	5	HEAST inhalation UR	TEF-based CSF (PAHs only)	

The output table of this query varies slightly between the *All Chemicals* and *Cumulative Exposure* options. These differences are illustrated in Exhibit 2-6 Both tables present the chemical name, CAS number, cancer toxicity data (UR, CSF, and WOE categories), calculated risk-based concentration, and information about the source of the toxicity data (source, year, and tier). The *All Chemicals* table also includes the exposure route (oral or inhalation) while the *Cumulative Exposure* table lists the medium (air, water, or food).

The presentation of the toxicity data also varies between *All Chemicals* and *Cumulative Exposure*. For *All Chemicals*, the table includes cancer slope factors (CSFs) in units of (mg/kg/day)⁻¹ for oral exposures, and unit risks (URs) in units of (μg/cu m)⁻¹ for inhalation exposures. The corresponding risk-based concentrations are presented in units of mg/kg/day and μg/cu m. For *Cumulative Exposure*, the table includes cancer slope factors (CSFs) in units of (mg/kg/day)⁻¹ for food exposures, and unit risks (URs) in units of (μg/cu m)⁻¹ for air exposures. For drinking water exposures, the table includes both CSFs in (mg/kg/day)⁻¹ and URs in μg/L that are calculated from CSFs.⁵ The risk-based concentration is presented in units of μg/cu m for

$$UR_{inh} \left(\mu g/cum\right)^{-1} = \frac{CSF_{oral} \left(mg/kg/day\right)^{-1} * 20cu\ m/day}{70kg * 1000\mu g/mg}$$

$$UR_{water} (\mu g/L)^{-1} = \frac{CSF_{oral} (mg/kg/day)^{-1} * 2L/day}{70kg * 1000\mu g/mg}$$

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⁴ The oral CSF is converted into an inhalation unit risk using the following equation, which assumes an inhalation rate of 20 cubic meters per day and an average body weight of 70 kilograms:

⁵ The conversion of the CSF to the UR assumes an ingestion rate of 2L of water per day and an average body weight of 70 kg. The following equation is used for the conversion:

air and μ g/L for drinking water. The risk-based value for food is presented as a dose in mg/kg/day that accounts for the total intake of a chemical through ingestion of various foodstuffs.

Exhibit 2-6			
CARCINOGENIC RISK-BASED CONCENTRATIONS BENCHMARKS REPORT OUTPUT			
All Chemicals	Cumulative Exposure		
chemical name	chemical name		
CAS number	CAS number		
exposure route (oral or inhalation)	medium (air, water, or food)		
cancer toxicity data (UR, CSF, and WOE)	cancer toxicity data (UR, CSF, and WOE)		
Oral: CSFs (mg/kg/day) ⁻¹	Food: CSFs (mg/kg/day) ⁻¹		
Inhalation: UR (µg/cu m) ⁻¹	Air: UR (μg/cu m) ⁻¹		
calculated risk-based concentration	Drinking Water: CSFs (mg/kg/day) ⁻¹ and UR (µg/L) ⁻¹		
Oral: (mg/kg/day)	calculated risk-based concentration		
Inhalation: (µg/cu m)	Food: (mg/kg/day)		
data source information (source, year, and tier)	Air: (μg/cu m)		
•	Drinking Water: (μg/L)		
	data source information (source, year, and tier)		

For both the *All Chemicals* and *Cumulative Exposure* options, the search presents a separate table summarizing for each tier the number of chemicals whose highest ranking data source comes from that tier. Only compounds with qualitative data are tabulated. Sample output from a *Cumulative Exposure/Water* search and an *All Chemicals/Oral* search (including Tier reports) are presented for comparison in Appendix D.

Toxic Equivalency Factor Slope Factors for PAHs - All Chemicals Option Only

Although current evidence suggests a WOE of B2, probable human carcinogen, for several polycyclic aromatic hydrocarbons (PAHs), insufficient data exist to quantify cancer potency benchmark values for these compounds. However, EPA has developed a set of coefficients, or toxic equivalency factors (TEFs) that compare the cancer potency of each of these PAHs to that of a reference PAH, benzo(a)pyrene. According to EPA, for example, the cancer potency of benzo(a)anthracene is one tenth that of benzo(a)pyrene. If the carcinogenic search does not find any oral values for a compound, it checks for a TEF for that compound and applies it to the IRIS oral cancer slope factor for benzo(a)pyrene. If both data are available, the search calculates a TEF-based slope factor and benchmark value for the compound (tier IIc).

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Chronic Non-carcinogenic Health Effect Benchmarks

This search presents toxicity benchmarks for non-cancer health effects associated with chronic exposure to pollutants (e.g., EPA Reference Doses or Concentrations). As with the cancer benchmark search, the user selects either the exposure route or media of interest and the search generates an output table of chronic non-carcinogenic health effect benchmark data for each chemical based on a hierarchy of data sources.⁶ The relative preference for the different chronic non-cancer benchmarks is shown in Exhibit 2-7.

The output table for this search presents the chemical name and CAS number, the type of benchmark, the benchmark value (in mg/kg/day for food and drinking water, and in mg/cu m for air), a description of the health effect on which the benchmark is based, the exposure route (or medium for the *Cumulative Exposure* option), and source information (tier and year). This search also produces a table summarizing the number of benchmarks presented from each tier of the data hierarchy. Sample output from the Chronic Non-Carcinogenic Benchmark search for a *Cumulative Exposure/air* search is presented in Appendix D.

Exhibit 2-7 DATA HIERARCHY FOR CHRONIC NON-CARCINOGENIC HEALTH EFFECT BENCHMARKS			
	Exposure Route		
Tier	Priority	Inhalation	Oral
Ι	1	IRIS Reference Concentration (RfC)	IRIS Reference Dose (RfD)
IIa	2	CAL EPA Reference Exposure Level (REL)	CAL EPA RfD
IIb	3	ATSDR Chronic Inhalation Minimal Risk Level (MRL)	ATSDR Chronic Oral Minimal Risk Level (MRL)

Acute Non-carcinogenic Health Effect Benchmarks

This search produces toxicity benchmarks related to non-cancer health effects associated with acute exposure to pollutants (e.g., ATSDR acute Minimum Risk Levels, or MRLs). The user selects the exposure route of interest (or medium for the *Cumulative Exposure* option) and the query provides an output table presenting non-carcinogenic health effect benchmark data pertaining to health effects resulting from acute exposures. The values presented for each chemical are selected based on a hierarchy of data sources.⁷ The relative preference for the different acute non-cancer benchmarks is shown in Exhibit 2-8.

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⁶ Caldwell et al., op. cit.

⁷ Caldwell et al., op. cit.

	Exhibit 2-8			
		ACUTE NON-CARCINOGENIC BENCHMA	ARKS DATA HIERARCHY	
		Exposu	re Route	
Tier	Priority	Inhalation	Oral	
Ι	1	IRIS Reference Concentration (RfC) for developmental effects only ¹	IRIS Reference Dose (RfD) for developmental effects only ¹	
IIa	2	EPA derived Levels of Concern (LOCs)/1000 ²	ATSDR acute oral Minimal Risk Level (MRL)	
IIb	3	ATSDR acute inhalation Minimal Risk Level (MRL)		
III	4	LC ₅₀	LD_{50}	

¹ Studies used to derive RfDs or RfCs for developmental effects typically involve very short exposure periods during gestation. These short exposures, on the order of several days, approximate acute exposures. Source: Caldwell, Jane C., Tracey J. Woodruff, Rachel Morello-Frosch, and Daniel A. Axelrad, "Application of Health Information to Hazardous Air Pollutants Modeled in EPA's Cumulative Exposure Project," *Toxicology and Industrial Health*, vol. 14, p. 429-54, 1998.

The output table for this query presents the chemical name and CAS number, the type of benchmark, the benchmark value (in mg/kg/day for food and drinking water, and in mg/cu m for air), a description of the health effect, the medium or exposure route, and the source information (citation for LD_{50} s and LC_{50} s, tier, and year). This query also produces a table summarizing the number of benchmarks presented from each tier of the data hierarchy. Sample output from the Acute Non-Carcinogenic Benchmark search for an *All Chemical/Oral and Inhalation* search is presented in Appendix D.

Summary of Toxicity Benchmark Values

The Summary of Toxicity Benchmark Values search produces a table of carcinogenic, non-carcinogenic chronic, and non-carcinogenic acute benchmarks for each chemical, based on the appropriate data hierarchies. If the *All Chemicals* option is chosen, the user can choose the exposure route for which data will be summarized (oral, inhalation, or both.) If the *Cumulative Exposure* option is selected, the user can choose the medium for which data will be summarized or can choose to display data for all media. If both exposure routes or all media are chosen, the search will produce multiple reports, one for each route or medium. Each summary output table will present the chemical name and CAS number, the carcinogenic risk-based concentration (corresponding to $1x10^{-6}$ risk), the chronic non-carcinogenic benchmark, and the acute non-carcinogenic benchmark. For each route or medium, this query also produces a table presenting the total number of data points in each tier of the cancer, non-cancer chronic, and non-cancer acute data hierarchies. Sample output for a Cumulative Exposure Study air summary search is presented in Appendix D.

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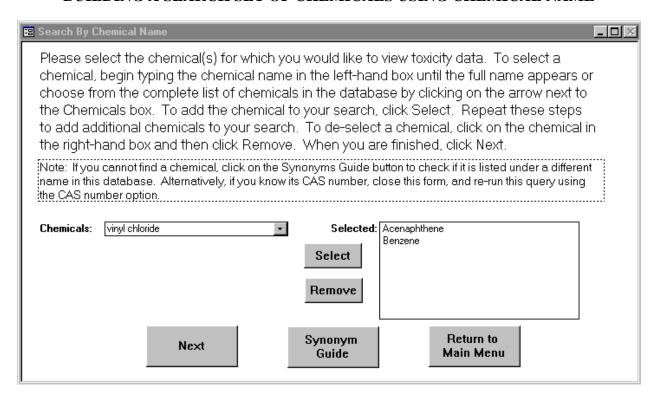
² LOCs are divided by 1000 because of concern over the peer review and supporting data for LOCs. Source: Caldwell et al., *op. cit*.

Search by Chemical

The Search by Chemical option allows the user to perform simple searches for toxicological data on one or more individual chemicals or on the chemical groups defined in the database. Initially, the user chooses to either define a set of individual chemicals for the search or to select from the 20 chemical groups defined in Appendix B. If the user selects the *Individual Chemicals* option, the user can build a search set using either chemical names or CAS numbers. Searching by CAS number is often more efficient than searching by chemical name, because while each chemical has only one CAS number that identifies it, it may be known by multiple names, only one of which has been used to identify it in the database. If the CAS number is not known, the user must know the specific name used to identify the chemical in the database in order to conduct a chemical name search. The Synonym Guide (see below) can assist the user in these situations. Exhibit 2-9 shows an example of selecting a set of chemicals using chemical names.

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Exhibit 2-9
BUILDING A SEARCH SET OF CHEMICALS USING CHEMICAL NAME



To select a set, choose a name (or CAS number or chemical group) by typing it into the box on the left or by clicking on the down arrow and selecting it from the pull-down menu. After choosing a chemical or group, click on the *Select* button to add it to the list. Repeat these steps to add more chemicals to the list. To remove a chemical, click on its name in the "Selected" box and then click *Remove*. When the list is complete, click on *OK*. If a particular chemical is not in the pull-down menu, it may be listed under a different synonym in the database. To check if it is in the database and find the chemical name it is listed under, click on *Synonym Guide*. This will activate the Synonym Guide search, which is described below. After checking the Synonym Guide, return to the chemical selection window and resume building the set.

After building a chemical or group set, select an exposure route (oral or inhalation) and then choose one of the following three report options, shown in Exhibit 2-10:

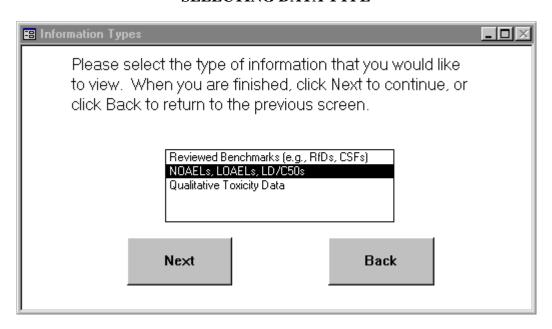
• **Reviewed Benchmarks.** This report can include CSFs, URs, RfDs, RfCs, MRLs, RELs, and/or LOCs that are available for the selected set of chemicals. The user can select one or more of these benchmarks to include in the report.

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⁸ See Appendix C for a glossary of acronyms used in the database.

- **LOAELs, NOAELs, and LD(LC)**₅₀**s.** This option creates a table of benchmark values from the primary literature as reported in the ATSDR *Toxicological Profiles* and *HAPs Profiles* (see Data Sources section). These data have not been peer reviewed to the extent of the *Reviewed Benchmarks* and should be used with this in mind. The user may choose to display NOAELs and LOAELs only, LD₅₀s or LC₅₀s only, or both (see Exhibit 2-11).
- Qualitative Toxicity Data. This option creates a table of qualitative toxicological information on health effects from EPA's *Health Effects Notebook (HAPfacts)*. Specifically, it reports potential health outcomes associated with chemical exposure, based on results of animal and human studies. No quantitative data are reported with this option.

Exhibit 2-10
SELECTING DATA TYPE

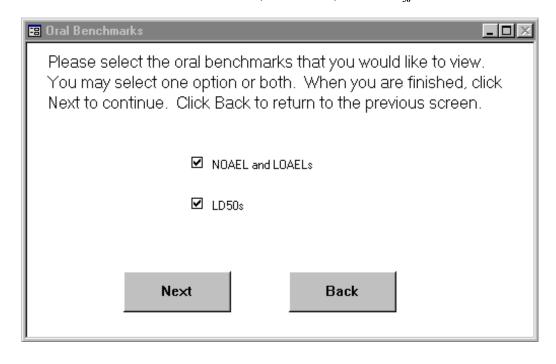


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⁹ See Appendix C for a glossary of acronyms used in the database.

Exhibit 2-11

SPECIFYING LOAELS, NOAELS, AND LD₅₀S



Exhibits 2-9 through 2-11 illustrate an example search for oral LOAELs, NOAELs, and LC₅₀s for acenaphthene, benzene, and vinyl chloride. Sample output from this search is presented in Appendix D. Output from a search for chronic EPA RfDs for the mercury chemical group (not shown) is also presented in Appendix D. This search returns RfDs for mercuric chloride, methyl mercury, and phenylmercuric acetate, each of which is included in the mercury chemical group.

Search by Health Effect

The Search by Health Effect option allows the user to create a table of toxicity data pertaining to specified types of health effects. The initial screen for this query presents the user with a list of health effect groupings from which to choose, as shown in Exhibit 2-12. The user selects one or more of these groupings and then selects an exposure route (oral, inhalation, or both; see Exhibit 2-13). Finally, the user selects the specific non-cancer benchmarks or data to present in the output table, if available, as shown in Exhibit 2-14. In order to retrieve data on all the chemicals in the database associated with a particular health effect, the user should select all of the data options on this screen. Exhibits 2-12 through 2-14 illustrate a search for chronic RfCs and RfDs related to cardiovascular and respiratory effects via oral and inhalation exposures.

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Exhibit 2-12

SELECTING HEALTH EFFECTS

Search by Health Effect		_ _ □ ×
		U.S. EPA Office of Policy
Searcl	h by Health Effe	ect
	cancer health effect(s) fo . You may select as ma , click Next.	-
☐ Auditory	☐ Immunological	
☐ Behavioral	☐ Metabolic	
☐ Body Weight	☐ Muscular	
✓ Cardiovascular	☐ Neurological	
☐ Death (LC/LD50s only)	☐ Ocular	Next
☐ Dermal	☐ Pancreatic	
☐ Developmental	☐ Renal	
☐ Endocrine	☐ Reproductive	Return to
☐ Exocrine	✓ Respiratory	Main Menu
☐ Gastrointestinal	☐ Skeletal	
☐ Hematological	☐ Splenic	
☐ Hepatic	☐ Systemic	

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Exhibit 2-13
SELECTING EXPOSURE ROUTE

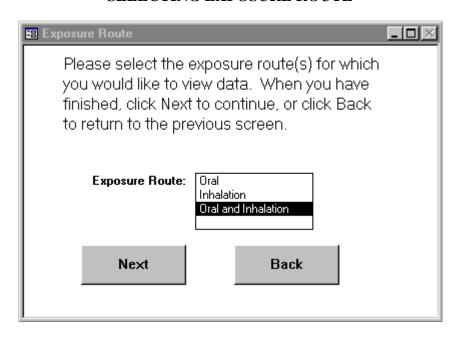


Exhibit 2-14
SELECTING BENCHMARKS

🔞 Oral and Inhalation Benchmarks	×
would like to view. You may	k Next to continue, or click Back
☑ Chronic RfD	□ гос
☑ Chronic RfC	□ NOAEL
☐ Subchronic RfD	□ LOAEL
☐ Subchronic RfC	☐ LC/LD50 (Death Only)
□ MRL	☐ Qualitative Information
□ REL	
Next	Back

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The output table will contain all the requested non-cancer data associated with the selected health effects groupings. If a chemical has both the liver (hepatic) and kidney (renal) effects, its health effect grouping would be hepatic/renal and would be included in a search for data on either hepatic or renal effects. The output table includes the chemical name and CAS number, the exposure route and type (acute, chronic), the type and value of the associated benchmark, details of the health effect, the data source, and the primary citation, if applicable. An example of the output from the search illustrated in Exhibits 2-12 through 2-14 is provided in Appendix D.

Synonym Guide

The Synonym Guide is included in the database to alleviate confusion arising from chemicals having multiple names. With only a few exceptions (see Appendix B) the database assigns only one name to each distinct CAS number. In some cases, the user may know a compound by a different name than the one appearing in the database. In such cases, the Synonym Guide can help the user locate the compound in the database. The guide contains over 5,000 synonyms obtained from the on-line *Hazardous Substances Data Bank* (HSDB) for the 344 chemicals in the database.

The Synonym Guide screen is shown below in Exhibit 2-15. To use the guide, simply begin typing the synonym in the *Synonyms* box at the top of the screen. As the name is typed, the program will attempt to complete the synonym with the nearest match to the letters typed. The user can also search a pull-down menu of synonyms by clicking the arrow to the right of the *Synonyms* box. Once the pull-down menu is activated, typing in the *Synonyms* box will scroll quickly down the list. For example, typing an initial "T" will scroll to the first synonym starting with "TE" and so on. The arrows to the right of the pull-down menu can also be used for scrolling.

Having selected a synonym, click the *Select* button to activate the guide. The chemical name used for the synonym in the database and its CAS number will appear in the appropriate boxes at the bottom of the screen. In Exhibit 2-15, a user looking for "1,1-dichloroethylene" has discovered that the database uses the name "vinylidene chloride" for this compound.

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¹⁰ Although the HSDB includes foreign synonyms as well as English synonyms, only English synonyms are included in the database.

Exhibit 2-15

SYNONYM GUIDE

😑 Synonym Gu	uide				_	
					U.S. EPA Office of Po	olicy
Synonyms:						•
	datab appea	ase, start typing ars. Then click (er will appear in nym Guide, click	with the chemical name use If the synonym into the Syno Select. The name used in t the boxes below. For more Ithe Help button. To see th	nyms box u he databas e informatio	intil the full name se and the CAS in about the	
		Select	Return to Previous Screen		Help	
Name in Data	abase:			CAS Number:		

Search Output

The tables generated by the searches described above can either be viewed on-screen, printed, or saved in Microsoft ExcelTM format. Enlarging the window by clicking on the *Maximize* button may aid in viewing the tables on-screen. The tables in the output window can be printed by selecting *Print* from the *File* menu.

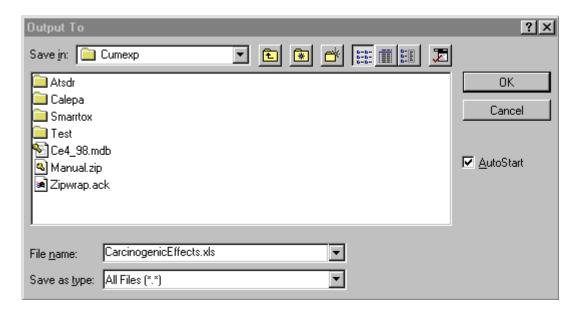
In certain cases, some of the data in fields with long entries (e.g., *Health Effects Descriptor*) may not be visible in the Microsoft AccessTM output format. If this is the case, or if a different data presentation is desired, the *Export to Excel*TM option is useful. Upon closing the output window, the user will be asked whether or not to save the output as an ExcelTM file. If the user chooses yes, the program asks for the directory where the file is to be saved and then saves the file, which can later be opened by Microsoft ExcelTM.

When selecting the directory where the ExcelTM file will be saved (Exhibit 2-16), pay attention to the *AutoStart* check box on the right side of the window. If there is a check in this box, the ExcelTM program will automatically open after saving the file. To save the file without opening ExcelTM at the same time, click on the *AutoStart* box to un-check it.

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Exhibit 2-16

EXPORTING TABLES TO EXCEL



Beyond the Interface

Users who have Microsoft Access[™] 7.0 have the added ability to by-pass the interface and explore the underlying tables directly. For users who are not familiar with Microsoft Access[™], we recommend against by-passing the interface. However, for more experienced users, working directly with the database allows the user to custom design queries for more specific data needs than those allowed by the user interface.

To by-pass the interface, choose *Close* from the *File* menu while the Main Menu is the active window. Behind the Main Menu is the *CEDBMMYY:Database* window which lists the tables, queries, forms, reports, macros, and modules that make up the Cumulative Exposure Toxicity Database. AccessTM can now be used to manipulate the database directly.

The pre-programmed searches in the Cumulative Exposure Toxicity Database were designed using a combination of queries, macros, and Visual BasicTM programming code that can be accessed from the *CEDBMMYY:Database* window or by right-clicking the buttons on the forms and choosing *Build Event*. Wherever possible, the macros and code contain comments to elucidate the query structure and provide signposts for individuals who wish to examine or modify the searches.

The searches also require many intermediate tables to function. These tables will either be hidden or will appear with a ghosted table symbol in the Tables window. If they are not visible, you can view them by changing the View settings in the AccessTM Options menu to show

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Hidden Objects. Any table whose name begins with an underscore, "_", is one of the core data tables. All other tables are intermediate tables used for storing data generated during the automated searches.

Users interested in modifying existing searches, creating their own queries, or simply exploring the underlying forms, macros, modules, and reports that comprise the user interface should consult Chapter 3 and Appendix E. Chapter 3 provides flow charts illustrating how each of the programmed searches function, and Appendix E lists all the components (macros, queries, etc.) associated with each search. Users can also refer to the built-in documentation in the macros and code for assistance. Users interested in learning how to design their own searches should consult an AccessTM manual and/or a guide to Visual BasicTM.

Troubleshooting

This section presents some common problems and suggested solutions.

1. *Oops! I accidentally closed the user interface window. How do I get it back?*

This problem applies to $Access^{TM}$ 7.0 users only. The Main Menu is a form entitled *AllReports*. In the *CEDBMMYY:Database* window on the screen, click on the *Forms* tab along the top of the window. Scroll all the way to the left, if you are not already there. The form listed in the upper left corner of the window is the *AllReports* form. Double-click on it and the interface Main Menu will reappear.

2. The database appears to be getting larger and I am running out of disk space. What can I do?

The database is a dynamic, not static, piece of software. While the database originally requires only about 7.5 MB of space on your hard disk drive, performing searches and otherwise using the database causes it to grow in size. ¹¹ Although most hard disk drives are large enough to easily accommodate the Cumulative Exposure Toxicity Database, if you are concerned about space, periodically compacting the database should help. To compact the database, close it (keeping AccessTM open). From the *Tools* menu, select *Database Utilities* and select *Compact Database* from the right hand menu. First locate the database to compact and click *Compact*. Then type the name of the compacted database (this must be different than the original database name, but you can rename it later) and click *Save*.

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¹¹ To perform queries and other database functions more quickly, AccessTM creates new temporary files, but does not later reclaim the space used by these files after it is finished with them. Thus, if the user performs a query several times, AccessTM uses new disk space each time, instead of rewriting over the same space.

3. The Benchmark searches aren't showing me all of the data.

There are three possible answers to this problem:

- a. The user ran a search using the *Cumulative Exposure* option, which limits the search to a subset of all of the chemicals in the database. Try running the search using the *All Chemicals* option.
- b. The Benchmark searches report the highest tier benchmark based on a hierarchy of data sources. The searches do not display additional values that may be available but that fall lower in the hierarchy. Try running the Search by Chemical program to generate a full list of available data for the desired chemicals.
- c. The chemical is not in the database, or no data are available. Check Appendix A or the Synonym Guide to verify that the chemical is in the database. If the database includes the chemical, but the Search by Chemical program does not report the data of interest, then the data are not in the database. Check Chapter 3 for the types of data included in the database.
- 4. The user interface windows don't fit on my screen.

The user needs to set the monitor resolution to 800 x 600 or greater. Screen resolution can be changed by selecting *Settings: Control Panels* from the *Start* menu, double clicking on *Display*, and selecting the *Settings* tab. For further information, the user should consult a guide to WindowsTM 95 or the user's guide for the monitor.

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This chapter presents more detailed technical background information regarding the Cumulative Exposure Toxicity Database structure, query design, and data sources. This information is intended for more advanced database users. While this information is not directly useful to Run-TimeTM users, who can only use the database through the user interface, it may provide helpful background information. More basic information about using the database is presented in Chapter 2.

This chapter is divided into three sections. The first presents an in-depth look at the structure and relationships of the data tables that comprise the database. The second presents flow charts that illustrate the steps involved in each pre-programmed search, including the macros, queries, and code on which they rely. The third section presents descriptions of the data sources used to develop the database.

DATABASE STRUCTURE

The structure of the Cumulative Exposure Toxicity Database is illustrated in Exhibit 3-1. As Exhibit 3-1 shows, the database is composed of nine primary tables, linked together by the *CAS Number* field.

Each of the basic tables will be discussed in-depth in this section. Below is a brief summary of the primary tables and the relationships between them.

- The General Information Table. This table serves to identify each compound in the database. The table lists each chemical's name and CAS number and indicates the media for which each was analyzed in the Cumulative Exposure Study.
- **Non-cancer and Cancer Tables.** These two tables contain toxicological data for non-carcinogenic and carcinogenic effects, respectively. In these tables, each chemical may have multiple records, each of which provides information associated with a specific health effect and/or benchmark.

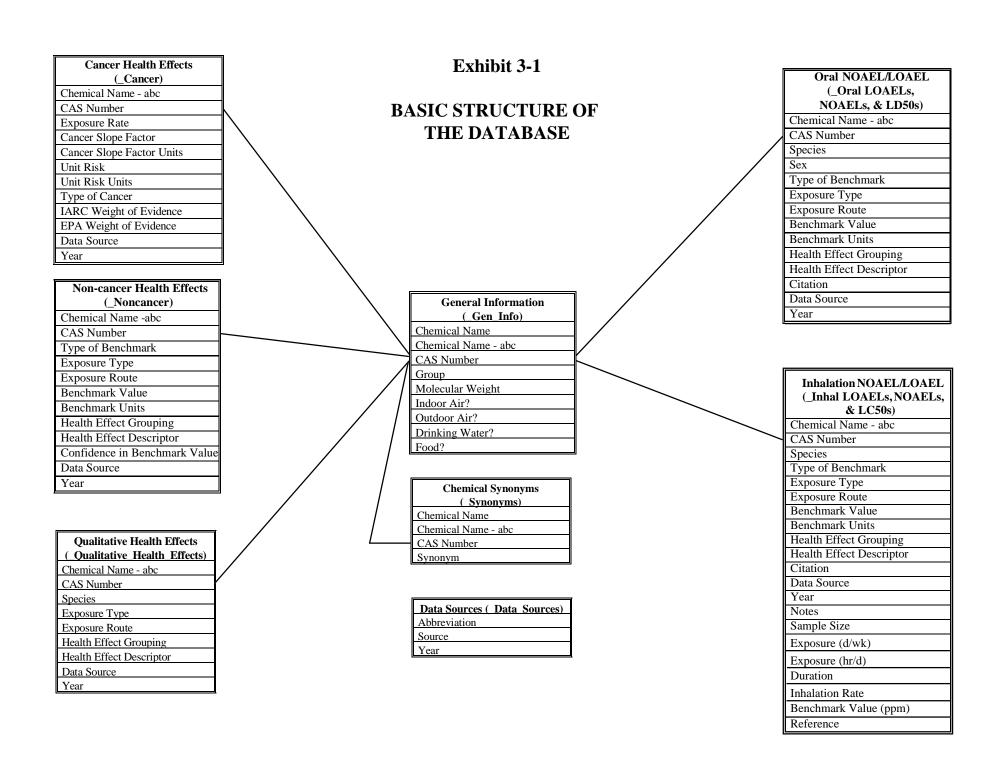
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- Oral NOAEL, LOAEL, & LD₅₀ Table and Inhalation NOAEL, LOAEL, & LC₅₀ Table. These tables present, for their respective exposure routes, toxicological data from various compendia of the primary literature. Specifically, these tables report No Observable Adverse Effects Levels (NOAELs), Lowest Observable Adverse Effects Levels (LOAELs), and either LD₅₀s (oral) or LC₅₀s (inhalation).
- **Qualitative Health Effects Table.** This table presents qualitative information on the range of non-cancer health effects associated with exposure to each chemical, as reported in EPA's *Health Effects Notebook for Hazardous Air Pollutants* (HAPfacts).
- **Synonyms Table.** This table lists synonyms for compounds in the database.
- **Toxic Equivalency Factors Table.** This table contains EPA's polycyclic aromatic hydrocarbon (PAH) toxic equivalency factors (TEFs), which compare the cancer potencies of several PAHs to that of a reference compound, benzo(a)pyrene.
- **Data Sources Table.** This table contains a list of the data sources used as the basis for the information presented in the other tables.

The main table at the center of Exhibit 3-1 is the General Information Table (_Gen_Info) Table, which identifies each compound in the database as well as whether or not it was studied in the various components of the Cumulative Exposure Study. All of the other tables, except the Data Sources Table, are linked to _Gen_Info using the CAS number that uniquely identifies each chemical. These links between tables allow the user to design queries that select, compare and compile specific information from different tables. For example, the user can easily specify both the non-cancer and cancer toxicity benchmarks for a given chemical and compare these data to estimated exposure levels. These links also enable the user to select data in one table based on criteria established in another table. For example, the user can select non-cancer toxicity data for all chemicals analyzed for air exposure in the Cumulative Exposure Study by using the *Outdoor Air?* field in the _Gen_Info Table and the toxicity data in the _Noncancer Table.

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¹ In a few cases where CAS numbers are not available, entries are assigned unique alphanumeric identifiers for internal use in the database. These identifiers are placed in the *CAS Number* field.



General Information Table

The General Information Table serves several functions in the database. As mentioned above, this table links nearly all the database tables together through the *CAS Number* field. In addition, as suggested by the title, the fields of this table contain basic information about each chemical, including its *Molecular Weight* and *CAS Number*. This table also includes four fields that identify the pathways for which EPA is developing exposure estimates as part of the Cumulative Exposure Study -- *Outdoor Air?*, *Drinking Water?* and *Food?*. Exhibit 3-2 lists the fields of the General Information Table and provides a brief description of each.

Each individual chemical included in the database has only one record in the _Gen_Info table which "identifies" it to the rest of the database. For some compounds, the database includes in _Gen_Info both a generic group entry (e.g., Lead and Compounds), and additional entries for individual chemicals within the group (e.g., lead acetate).

Exhibit 3-2				
	GENERAL INFORMATION TABLE			
Field Name	Field Description	Specified Field Characteristics		
Chemical Name	Name of chemical.	Text of 30 characters		
Chemical Name - abc	Name of chemical formatted with prefixes at the end.	Text of 55 characters. The database does not allow the user to leave this field blank.		
CAS No.	CAS number of the chemical. If a CAS number was not available, a unique alphanumeric identifier was assigned to the chemical or group and is shown here.	Text of 15 characters. The database does not allow the user to leave this field blank.		
Group	Identifies the chemical group to which a compound belongs, if any.	Text of 25 characters		
Molecular Weight	Molecular weight of the chemical. This information can be used for conversions between ppm and $\mu g/cu$ m.	Number		
Outdoor Air?	Identifies those chemicals included in the outdoor air pollution analysis of the Cumulative Exposure Study.	Yes or No		
Drinking Water?	Identifies those chemicals included in the drinking water analysis of the Cumulative Exposure Study.	Yes or No		
Food?	Identifies those chemicals included in the food contamination analysis of the Cumulative Exposure Study.	Yes or No		

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The generic entry and the individual compounds are linked together by the *Group* field in _Gen_Info, which indicates the name of the group to which a compound belongs. A user can thus find toxicological information for all lead compounds included in the database by querying all compounds whose *Group* is lead.

Cancer Health Effects Table

The Cancer Health Effects (_Cancer) Table provides data on the carcinogenicity of pollutants in the database. In general, each record in the cancer table provides a measure of cancer potency for a given chemical and exposure route, and information associated with that measure. Some records, however, contain information about a chemical's carcinogenicity (such as weight of evidence classification), but do not provide a cancer potency measure because such measures have not been established. A chemical will have more than one record in this table if it has more than one cancer potency measure. Exhibit 3-3 presents a description of each of the fields in the table.

The measures of carcinogenic potency included in the database (i.e., cancer slope factors and unit risks) are based on EPA's IRIS and HEAST databases, and data from the California EPA. Cancer slope factors (CSFs) indicate the risk associated with a given oral dose (i.e., risk per mg/kg/day of ingested pollutant). Inhalation unit risk (UR) values measure of the risk per concentration unit (i.e., the risk per μ g/cu m of pollutant in the air). The UR values can be used to derive airborne contaminant concentrations associated with particular benchmark risk levels (e.g., one-in-a-million or 1×10^{-6}). These benchmark concentrations can then be used to evaluate the significance of potential exposures to contaminants. In addition, the table provides information on the weight of evidence (WOE) that a chemical is carcinogenic, as classified by EPA and the International Agency for Research on Cancer (IARC). Exhibit 3-4 describes each agency's weight of evidence scale, and Exhibit 3-5 presents the data sources used to obtain key data elements for the Cancer Health Effects Table. The *Data Sources* section of this chapter provides more information about each source.

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Exhibit 3-3			
CARCINOGENIC EFFECTS TABLE			
Field Name	Field Description	Field Characteristics	
Chemical Name-abc	Name of chemical formatted with root first and prefixes after.	Text of 55 characters. The database does not allow the user to leave this field blank.	
CAS No.	Chemical Abstract Number or other unique alphanumeric identifier.	Text of 50 characters. The database does not allow the user to leave this field blank.	
Exposure Route	Route of exposure (i.e., inhalation or oral).	Text of 12 characters. The user may only enter the words "oral," "inhalation," or "unspecified." Default is the word "unspecified."	
Cancer Slope Factor	Value of the specified cancer slope factor (CSF). If Weight of Evidence information is available, but a cancer slope factor is not available, this field will be blank.	Number.	
Cancer Slope Factor Units	Specified units of the cancer slope factor. The units are (mg/kg/day) ⁻¹ for oral exposures.	Text of 50 characters.	
Unit Risk	The risk associated with one concentration unit of an airborne contaminant.	Number.	
Unit Risk Units	The units associated with the unit risk value for airborne contaminants, (µg/cu m) ⁻¹ .	Text of 50 characters.	
Type of Cancer	Type of cancer associated with the cancer slope factor or unit risk, or with exposure if a toxicity value is not provided.	Text of 225 characters.	
IARC Weight of Evidence	Carcinogenic Weight of Evidence (WOE) as developed by IARC.	Text of 4 characters.	
EPA Weight of Evidence	Carcinogenic Weight of Evidence (WOE) as developed by EPA.	Text of 4 characters.	
Data Source	The information source used to obtain the data in the record (e.g., IRIS, HEAST).	Text of 25 characters. Every record in the database must have an entry in this field.	
Year	Year of the data source from which the associated information was taken.	Text of 10 characters.	

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Exhibit 3-4			
DESCRI	DESCRIPTION OF EPA AND IARC WEIGHT OF EVIDENCE CLASSIFICATIONS		
EPA	IARC	Description of Category	
A	1	Human carcinogen	
B1	2A	Probable human carcinogen limited human evidence	
B2	2A	Probable human carcinogen sufficient evidence in animals and inadequate or no evidence in humans	
С	2B	Possible human carcinogen	
D	3	Not classifiable as to human carcinogenicity	
Е	4	Evidence of noncarcinogenicity for humans	

Exhibit 3-5		
CANCER POTENCY MEASURES AND THE CORRESPONDING DATA SOURCES		
Type of Toxicity Value Data Source		
Cancer Slope Factor (CSF)	IRIS, HEAST, or Cal EPA	
Unit Risk (UR)	IRIS, HEAST, or Cal EPA	
Weight of Evidence (WOE)	IRIS, IARC, 112(g)	

Non-cancer Health Effects Table

The Non-cancer Health Effects Table of the database includes information on the chronic, subchronic, and acute health effects associated with both oral and inhalation exposure. As shown in Exhibit 3-6, the information contained in each record pertains to a given toxicity benchmark. The fields of each record provide the following information about each benchmark value:

- The type of exposure associated with the toxicity benchmark value. There are two fields in the database that characterize the type of exposure: *Exposure Type* (acute, chronic, or subchronic) and *Exposure Route* (either inhalation or oral).
- The non-cancer toxicity benchmark. The *Type of Toxicity Benchmark* field specifies the name of the benchmark (e.g., MRL, RfD, RfC, etc.), and the *Toxicity Benchmark Value* field provides the numerical value of the benchmark. The *Benchmark Units* field provides the units associated with the benchmark (e.g., mg/kg/day for an RfD). In addition, the *Data Source* field identifies the source of the benchmark value. Exhibit 3-7

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shows each type of toxicity benchmark presented in the non-cancer table along with the data sources used to obtain the value. Each data source is described in the *Data Sources* section of this chapter.

Exhibit 3-6			
NON-CANCER HEALTH EFFECTS TABLE			
Field Name Field Description Field Characteris			
Chemical Name-abc	Name of chemical formatted with root first and prefixes after.	Text of 55 characters. The database does not allow the user to leave this field blank.	
CAS No.	CAS number, or other unique identifier, for the chemical.	Text of 15 characters. The database does not allow the user to leave this field blank.	
Type of Benchmark	Identification of the type of toxicity benchmark (i.e. RfD, RfC, Sub-RfD, Sub-RfC, REL, MRL, LOC).	Text of 12 characters. The default for this field is the word "unspecified." The default is used for records that provide information on other health effects not associated with benchmark values.	
Exposure Type	Type of exposure associated with the toxicity benchmark value (i.e., acute, chronic, or subchronic).	Text of 11 characters. Default for this field is the word "unknown." The user may only enter the words "acute," "chronic," "subchronic," or "unknown" in this field.	
Exposure Route	Route of exposure (i.e., inhalation or oral) associated with the toxicity benchmark.	Text of 12 characters. The user may only enter the words "oral," "inhalation," or "unspecified." Default is the word "unspecified."	
Benchmark Value	The value of the specified toxicity benchmark for the specified type of exposure and route of exposure.	Number.	
Benchmark Units	Units for the toxicity benchmark value. (e.g., mg/kg/day, µg/cu m).	Text of 50 characters.	
Health Effect Grouping	Category assigned to each health effect. These categories generally relate to the target organ or system, with groupings such as hepatic, renal, respiratory, etc.	Text of 50 characters. Default is the word "unspecified."	
Health Effect Descriptor	Health effect associated with the benchmark value. This field contains more detailed information on the health effect than the health effect grouping field, describing the specific effect associated with exposure.	Text of 255 characters. Default is the word "unspecified."	
Confidence in	Confidence value assigned by the	Text of 10 characters. Not all benchmarks	
Benchmark Value	organization that developed the benchmark.	have associated confidence values.	
Data Source	The information source used to obtain the data in the record (e.g., IRIS, HEAST).	Text of 20 characters. Every record in the database must have an entry in this field.	
Year	Year of the data source from which the associated information was taken.	Text of 10 characters.	

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• The health effects associated with the benchmark value. Two fields in the Non-cancer Health Effects Table are devoted to providing health effect information. These are the *Health Effect Descriptor* field, which describes the health effect associated with the benchmark value, and the *Health Effect Grouping* field which categorizes the health effect according to target organ or system.

Exhibit 3-7 TYPES OF NON-CANCER TOXICITY BENCHMARK VALUES AND THE CORRESPONDING DATA SOURCES			
Type of Toxicity Value Abbreviation Data Source			
Level of Concern	LOC	112(G) and EHS	
Minimal Risk Level	MRL	ATSDR	
Reference Concentration	RfC	IRIS and HEAST	
Reference Dose	RfD	IRIS, HEAST and Cal EPA	
Reference Exposure Level	REL	Cal EPA	
Subchronic Reference Concentration	Sub-RfC	HEAST	
Subchronic Reference Dose	Sub-RfD	HEAST	

Qualitative Health Effects Table

The Qualitative Health Effects Table contains qualitative information on the range of non-cancer health effects associated with exposure to each chemical, including those for which there are no benchmark values. The data in this table are obtained from EPA's *Health Effects Notebook for Hazardous Air Pollutants* (HAPfacts).² HAPfacts provides chemical fact sheets of toxicity information for each of the Hazardous Air Pollutants specified in the Clean Air Act Amendments of 1990. Each fact sheet provides a qualitative summary of health effects that have been reported for a specific chemical.

The structure of the Qualitative Health Effects Table is similar to the Non-cancer Health Effects Table with two exceptions. First, a field, named Species, indicates the species (e.g., human, rat, hamster) in which each health effect has been observed. Second, the Qualitative Health Effects Table does not include fields referring to specific benchmarks (i.e., Benchmark Value, Benchmark Units, and Confidence in Benchmark Value), because it does not contain specific benchmark values. Exhibit 3-8 describes the contents and characteristics of each field in this table.

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² U.S. Environmental Protection Agency, *Health Effects Notebook for Hazardous Air Pollutants*, December 1994.

Exhibit 3-8			
QUALITATIVE HEALTH EFFECTS TABLE			
Field Name	Field Description	Field Characteristics	
Chemical Name - abc	Name of chemical formatted with root first and prefixes after.	Text of 55 characters. The database does not allow the user to leave this field blank.	
CAS Number	Chemical Abstract number of the chemical.	Text of 15 characters. The database does not allow the user to leave this field blank.	
Species	Species in which health effect was observed.	Text of 25 characters. The database does not allow the user to leave this field blank.	
Exposure Type	Type of exposure associated with the health effect (i.e., acute, chronic, or unknown).	Text of 11 characters. The default for this field is the word "unknown."	
Exposure Route	Route of exposure associated with the health effect (i.e., inhalation, oral, or unspecified).	Text of 12 characters.	
Health Effect Grouping	Category assigned to each health effect. These categories generally relate to the target organ or system (e.g., hepatic, respiratory, cardiovascular, etc.).	Text of 65 characters. Default is "unspecified."	
Health Effect Descriptor	Health effect associated with the benchmark value. This field provides more detailed information on the health effect than the <i>Health Effect Grouping</i> field.	Text of 255 characters. Default is "unspecified."	
Data Source	The information source used to obtain the data in the record.	Text of 20 characters. The database does not allow the user to leave this field blank.	
Year	Year of the data source from which the associated information was taken.	Text of 10 characters.	

Oral NOAEL/LOAEL Table

The Oral NOAEL/LOAEL Table provides three types of toxicity data: NOAELs, LOAELs, and LD₅₀s. NOAEL, or "no observable adverse effect level," is the level determined from a toxicity study to be the highest exposure concentration (or dose) at which a specific adverse health effect was not observed. LOAEL, or "lowest observable adverse effect level," represents the lowest exposure concentration (or dose) at which an adverse health effect was observed in a toxicity study. LD₅₀s are doses that have been reported to be lethal in fifty percent of a study's test sample. All of the toxicity data included in the Oral NOAEL/LOAEL Table are from the Toxicological Profiles developed by the Agency for Toxic Substances and Disease Registry.³

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³ Agency for Toxic Substances and Disease Registry, *Toxicological Profiles on CD-ROM*, CRC Press, Inc., 1997.

The structure of the Oral NOAEL/LOAEL Table is described in Exhibit 3-9. This structure is similar to that used for the Non-cancer Health Effects Table; however, there are three additional fields. The *Species* field lists the species (e.g., human, rat, monkey) that was tested. The *Sex* field indicates if the study or observed effects were limited to only males or females. If the toxicity data apply to both sexes or the sex was not specified, then the sex field is left blank. The third additional field is named *Citation*, and is used to cite the original study in which the data were reported. This field is different than the *Data Source* field, which refers to the secondary source from which the data were obtained.

Inhalation NOAEL/LOAEL Table

The Inhalation NOAEL/LOAEL Table is similar to the Oral NOAEL/LOAEL Table, providing NOAELs, LOAELs, and LC₅₀s for inhalation exposures. All of the data in this table come from EPA's Hazardous Air Pollutant Profiles (HAPs Profiles) or ATSDR's Toxicological Profiles.⁴

Exhibit 3-10 describes the structure and data fields of the Inhalation NOAEL/LOAEL Table. The modified structure is similar to that used for the Oral NOAEL/LOAEL Table, but it has additional fields that provide information about the exposure conditions (*Sample Size*, *Exposure* (*d/wh*); *Exposure* (*hr/d*), *Duration*, and *Inhalation Rate*).

In addition, the table contains a field named *Notes*. This field contains numerical references to notes in the hard copy of the HAPs Profiles. The actual notes provide information about the studies on which the toxicity values are based, and as such allow the user to judge the reliability and quality of the data. Based on the notes in HAPs Profiles, data from some studies were not entered into the database because they were clearly inappropriate for the purposes of this database. (See the *Data Sources* section of this chapter for more information.) However, data from the remaining studies were entered but have not been extensively reviewed for more ambiguous or subtle quality issues. Database users may wish to consult the notes in the HAPs Profiles document (as referenced in the *Notes* field) to ensure that the quality of individual studies is adequate for their needs. The actual text of the notes is not present in the Cumulative Exposure Toxicity Database, because the large number of notes and the independent nature of the note numbering scheme precluded their inclusion.

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⁴ U.S. Environmental Protection Agency, *Hazardous Air Pollutants: Profiles of Non-cancer Toxicity from Inhalation Exposures*, September 1993; and Agency for Toxic Substances and Disease Registry, *Toxicological Profiles on CD-ROM*, CRC Press, Inc., 1997.

Exhibit 3-9			
ORAL NOAEL/LOAEL TABLE			
Field Name	Field Description	Field Characteristics	
Chemical Name - abc	Name of chemical formatted with root first and prefixes after.	Text of 55 characters. The database does not allow the user to leave this field blank.	
CAS Number	Chemical Abstract number of the chemical.	Text of 15 characters. The database does not allow the user to leave this field blank.	
Species	Species in which health effect was observed.	Text of 25 characters. The database does not allow the user to leave this field blank.	
Sex	Sex that either was exposed to chemical or experienced effect (i.e., male or female). Blank if a single sex was not indicated.	Text of 11 characters.	
Type of Benchmark	Identification of the type of toxicity benchmark (i.e., LD ₅₀ , NOAEL, or LOAEL).	Text of 12 characters.	
Exposure Type	Type of exposure associated with the health effect (i.e., acute, subchronic, or chronic).	Text of 11 characters. Default is "unknown."	
Exposure Route	Route of exposure associated with the health effect (i.e., oral).	Text of 12 characters.	
Benchmark Value	The value of the specified toxicity benchmark for the specified type and route of exposure.	Number. Default is "-9.99E-99."	
Benchmark Units	Units of the toxicity benchmark value (i.e., mg/kg/day).	Text of 50 characters.	
Health Effect Grouping	Category assigned to each health effect. These categories generally relate to the target organ or system (e.g., hepatic, respiratory, cardiovascular, etc.).	Text of 50 characters. Default is "unspecified."	
Health Effect Descriptor	Health effect associated with the benchmark value. This field provides more detailed information on the health effect than the <i>Health Effect Grouping</i> field.	Text of 255 characters. Default is "unspecified."	
Citation	Original study in which results were reported.	Text of 55 characters. The database does not allow the user to leave this field blank.	
Data Source	The information source used to obtain the data in the record (e.g., ATSDR Toxicological Profiles).	Text of 20 characters. The database does not allow the user to leave this field blank.	
Year	Year of the data source from which the associated information was taken.	Text of 10 characters.	

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Exhibit 3-10			
INHALATION NOAEL/LOAEL TABLE			
Field Name	Field Description	Field Characteristics	
Chemical Name -	Name of chemical formatted with root first	Text of 50 characters. The database does not	
abc	and prefixes after.	allow the user to leave this field blank.	
CAS Number	Chemical Abstract number of the chemical.	Text of 15 characters. The database does not allow the user to leave this field blank.	
Species	Species in which health effect was observed.	Text of 25 characters. The database does not allow the user to leave this field blank.	
Type of	Identification of the type of toxicity	Text of 12 characters. The database does not	
Benchmark	benchmark (i.e., LD ₅₀ , NOAEL, or LOAEL).	allow the user to leave this field blank.	
Exposure Type	Type of exposure associated with the health effect (i.e., acute, subchronic, or chronic).	Text of 11 characters. Default is "unknown."	
Exposure Route	Route of exposure (i.e., inhalation) associated with the health effect.	Text of 12 characters.	
Benchmark Value	The value of the specified toxicity benchmark for the specified type and route of exposure.	Number. Default is "-9.99E-99."	
Benchmark Units	Units of the toxicity benchmark value (i.e., mg/cu m).	Text of 50 characters.	
Health Effect	Category assigned to each health effect.	Text of 50 characters. Default is	
Grouping	These categories generally relate to the target organ or system (e.g., hepatic, respiratory, cardiovascular, etc.).	"unspecified."	
Health Effect	Health effect associated with the benchmark	Text of 255 characters. Default is	
Descriptor	value. This field provides more detailed information on the health effect than the <i>Health Effect Grouping</i> field.	"unspecified."	
Citation	Original study in which results were reported.	Text of 60 characters. The database does not allow the user to leave this field blank.	
Data Source	The information source used to obtain the	Text of 20 characters. The database does not	
	data in the record (e.g., HAPs Profiles)	allow the user to leave this field blank.	
Year	Year of the data source from which the associated information was taken.	Text of 10 characters.	
Notes	Numerical references from HAPs Profiles for notes about the record.	Text of 23 characters.	
Sample Size	Number of individuals exposed.	Text of 7 characters.	
Exposure (d/wk)	Number of days per week of exposure.	Text of 4 characters.	
Exposure (hr/d)	Number of hours per day of exposure.	Text of 4 characters.	
Duration	Number of days, weeks, months, or years over which exposure occurred.	Text of 8 characters.	
Inhalation Rate	Rate of inhalation for the test population.	Number	
Benchmark (ppm)	The value of the toxicity benchmark given in parts per million.	Number	
Reference	Numerical references from HAPs Profiles concerning the sources used by HAPs Profiles to obtain the data.	Text of 6 characters.	

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Chemical Synonym Table

While only one CAS number exists for each chemical, many compounds are known by multiple names. In fact, separate components of the Cumulative Exposure Study sometimes refer to the same chemical using different names. The database assigns a single name to each unique chemical. Therefore, the chemical names used in the Cumulative Exposure Toxicity Database do not always agree with the names used in other sources for the same compounds. The Chemical Synonym Table lists other names that may be used for the compounds in the database. The list of synonyms was obtained from the National Library of Medicine's Hazardous Substances Data Bank (HSDB).⁵ The Chemical Synonym Table is useful in eliminating the confusion caused by multiple names. Exhibit 3-11 describes the structure of this table. Each record lists one synonym. Thus, a chemical with twenty possible names has twenty separate records in the table.

Exhibit 3-11			
CHEMICAL SYNONYM TABLE			
Field Name	Field Description	Field Characteristics	
Chemical Name	Name of chemical.	Text of 55 characters. The database does not allow the user to leave this field blank.	
Chemical Name - abc	Name of chemical formatted with root first and prefixes after.	Text of 55 characters. The database does not allow the user to leave this field blank.	
CAS Number	Chemical Abstract number of the chemical.	Text of 15 characters. The database does not allow the user to leave this field blank.	
Synonym	Other name for the compound	Text of 255 characters.	

Toxic Equivalency Factors Table

Cancer risk-based concentration benchmark values have not been developed for most polycyclic aromatic hydrocarbon (PAH) compounds. EPA has developed coefficients, or toxic equivalency factors (TEFs), that compare the cancer potencies of several of these compounds to that of a reference compound, benzo(a)pyrene. The Toxic Equivalency Factors Table of the database contains the available EPA TEF data. This information is useful for calculating cancer benchmarks for PAHs that lack better cancer toxicity data. Exhibit 3-12 describes the structure of this table.

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⁵ U.S. National Library of Medicine, TOXNET, Hazardous Substances Data Bank, accessed December 1997.

Exhibit 3-12				
	TOXIC EQUIVALENCY FACTOR TABLE			
Field Name	Field Description	Field Characteristics		
Chemical Name - abc	Name of chemical formatted with root first and prefixes after.	Text of 55 characters.		
CAS Number	Chemical Abstract number of the chemical.	Text of 15 characters. The database does not allow the user to leave this field blank or to have duplicate entries.		
Chemical Group	Identifies the chemical group to which the chemical belongs (i.e., polycyclic organic matter).	Text of 25 characters.		
TEF	Toxic equivalency factor (i.e., cancer potency relative to benzo(a)pyrene).	Number.		
Reference	Citation for study on which the TEF is based.	Text of 255 characters.		
Source	Source of the TEF data (i.e., EPA TEF).	Text of 10 characters.		

DATABASE SEARCHES

The Cumulative Exposure Toxicity Database's user interface offers seven programmed data searches. These searches allow users to obtain information from the database easily and with minimal knowledge of Microsoft Access™. This section provides flow charts (Exhibits 3-13 through 3-19) for each of the seven search programs. The flow charts depict the functioning of the user interface in detail, and provide a generalized description of each search's underlying macros and Visual Basic™ code. This section is useful for understanding the available user options, learning the names of specific interface windows and program macros, and understanding the basic structure of the search programs.

The flow charts do not diagram each individual program step. Instead, they provide an overview of the programs by combining similar macros and sets of queries together to show the general program structures. Users should refer to Chapter 2 for more information about the search options and data hierarchies. Appendix E provides a complete listing of the components (i.e., tables, forms, queries, reports, macros, and modules) used by each search. Appendix E and the flow charts provide users with a starting point for further exploration of individual searches.

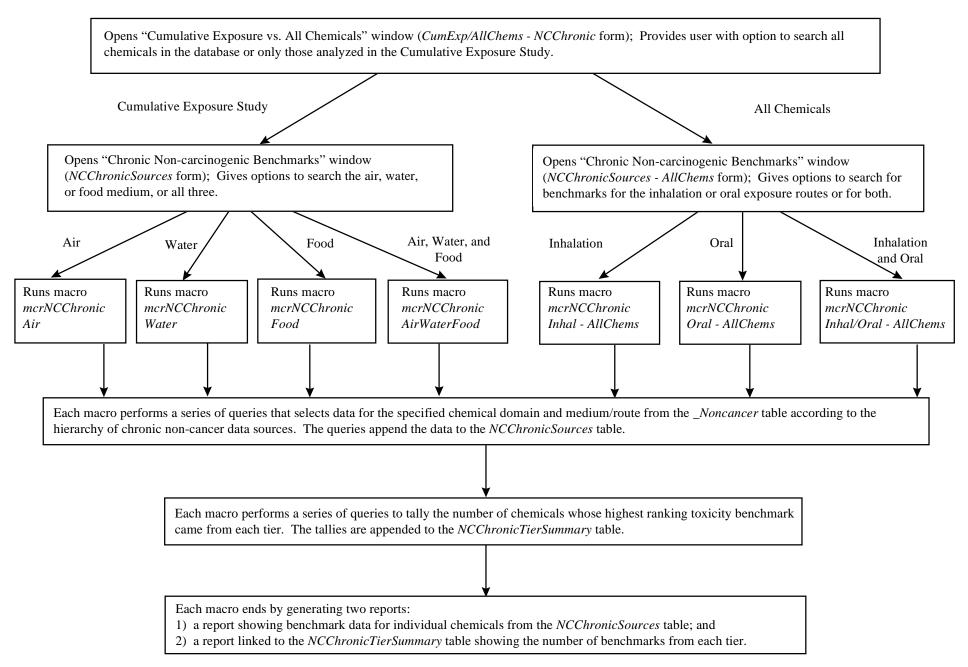
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CARCINOGENIC RISK-BASED CONCENTRATION BENCHMARK SEARCH

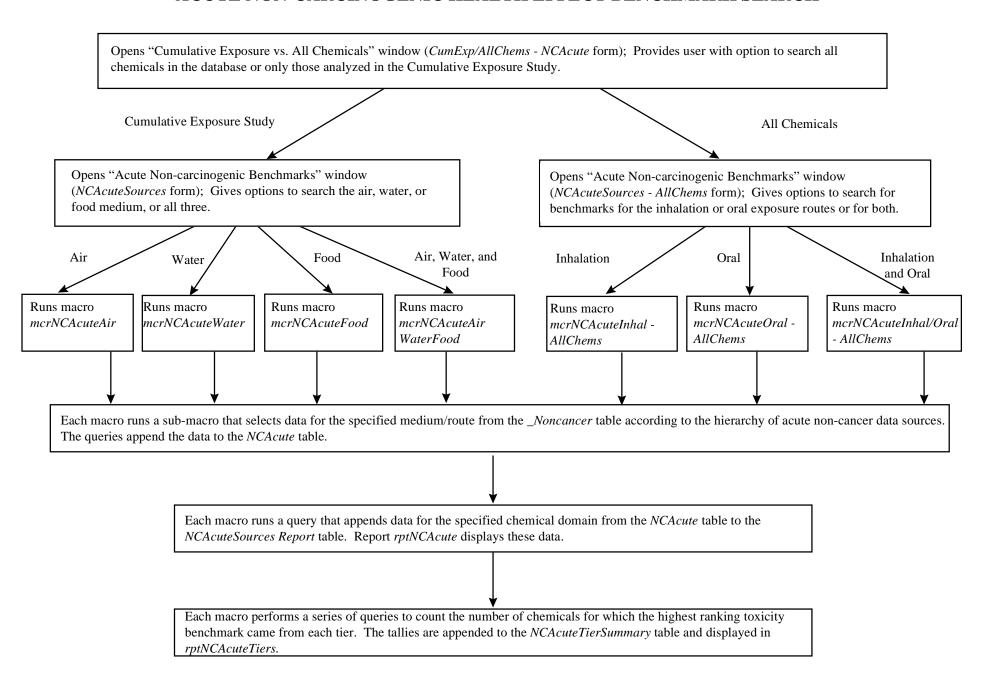
Opens "Cumulative Exposure vs. All Chemicals" window (CumExp/AllChems - Cancer form); provides user with option to search all chemicals in the database or only those analyzed in the Cumulative Exposure Study. Cumulative Exposure Study All Chemicals Opens "Carcinogenic Risk-Based Concentration Benchmarks" Opens "Carcinogenic Risk-Based Concentration Benchmarks" window (CancerHealth form); Gives options to search the air, window (CancerHealth - AllChems form); Gives options to search water, or food medium, or all three. for benchmarks for the inhalation or oral exposure routes or for both. Air, Water, and Air Water Food Inhalation Oral Inhalation Food and Oral Runs macro CreateAirCancer CreateWaterCancer CreateFoodCancer CreateAir/Water/ CreateInhalCancer CreateOralCancer CreateOral/Inhal **HealthTable** HealthTable *HealthTable* FoodCancerHealth. HealthTable -HealthTable -CancerHealthTable -Table AllChems AllChems AllChems Each macro performs a sub-macro to select data for the specified medium/route from the Cancer table according to the hierarchy of cancer data sources. If no quantitative data are available from the hierarchy of data sources, the macros search for a weight of evidence. The queries append the data to the CancerSources table. Each macro performs multiple queries to select data from Cancer Sources table for the specified chemical domain, calculate risk-based concentrations, and append records to the CancerSourcesReport table. Each macro performs a series of queries to tally the number of chemicals whose highest ranking toxicity benchmark came from each tier. The tallies are appended to the *TierSummary* table. Each macro ends by generating two reports: 1) a report showing benchmark data for individual chemicals from the CarcinogenicEffects table; and

2) a report linked to the *TierSummary* table showing the number of benchmarks from each tier.

CHRONIC NON-CARCINOGENIC HEALTH EFFECT BENCHMARK SEARCH



ACUTE NON-CARCINOGENIC HEALTH EFFECT BENCHMARK SEARCH



SUMMARY OF TOXICITY BENCHMARK VALUES SEARCH

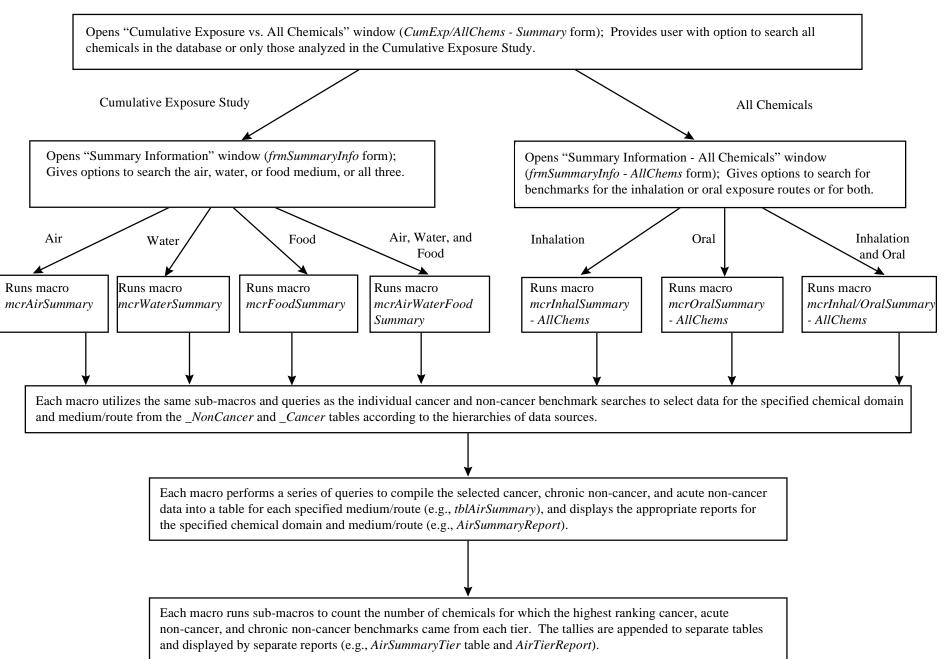
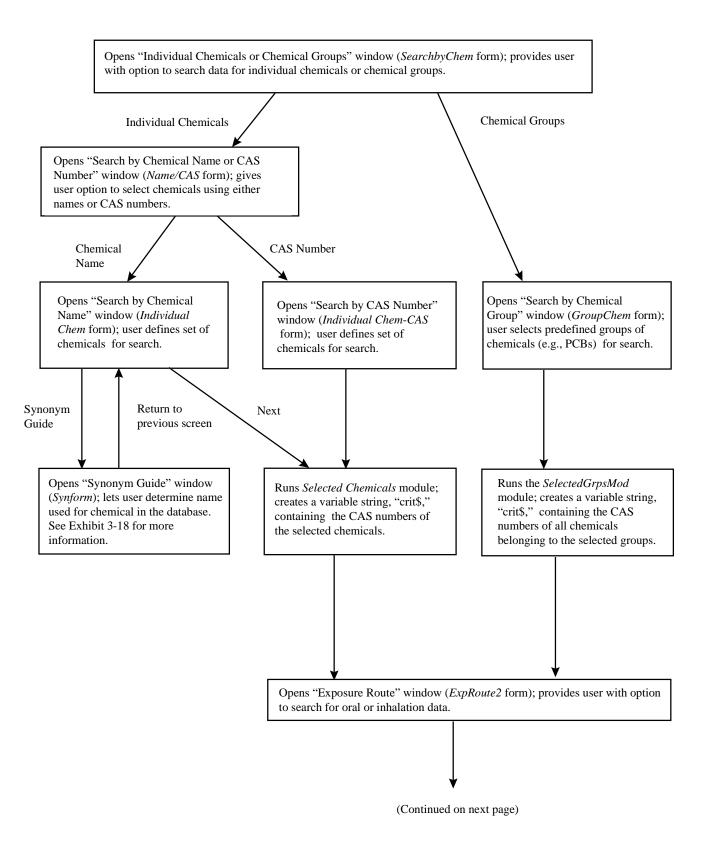
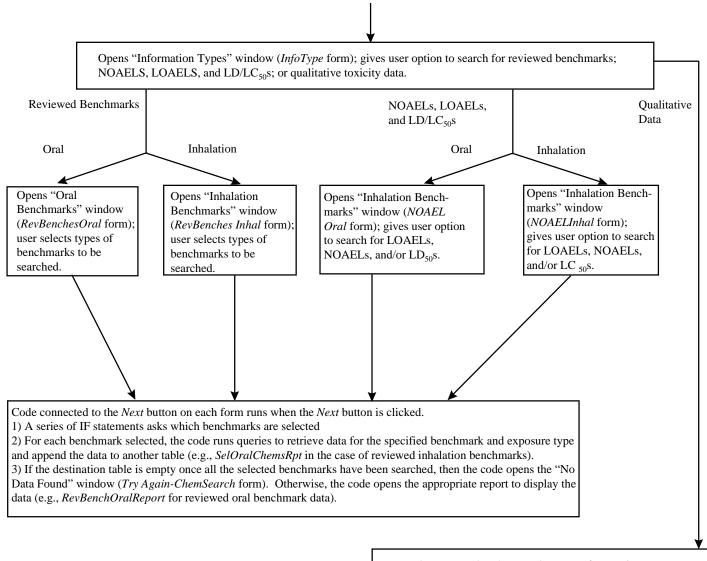


Exhibit 3-17 SEARCH BY CHEMICAL



SEARCH BY CHEMICAL

(Continued from previous page)

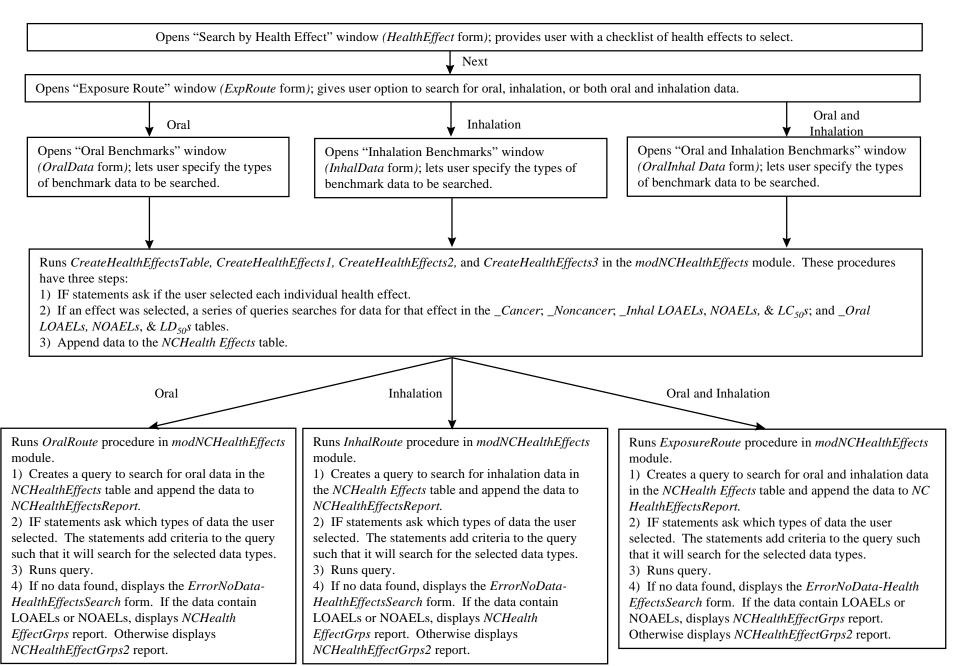


Runs code connected to the Next button on form *InfoType*.

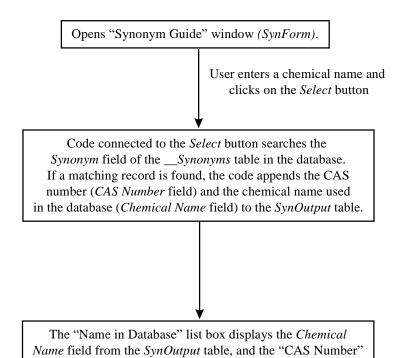
1) Code searches the *_Qualitative _Health_Effects* table for either oral or inhalation data for chemicals in the variable string "crit\$".

2) Depending on the exposure route, the code appends data to either the *QualOral* or *QualInhal* table and displays the data in *QualOralReport* or *QualInhalReport*.

Exhibit 3-18 SEARCH BY HEALTH EFFECT



SYNONYM GUIDE



list box shows the CAS Number field.

DATA SOURCES

This section summarizes the data sources used to develop the Cumulative Exposure Toxicity Database. The database is derived from secondary data sources that contain toxicological benchmarks, potency measures, and other health effects information for pollutants included in the Cumulative Exposure Study. The following sources provided information in the database:

- EPA Integrated Risk Information System (IRIS);
- EPA Health Effects Assessment Summary Tables (HEAST);
- EPA Levels of Concern (LOCs) for SARA Title III Extremely Hazardous Substances:
- EPA Clean Air Act Section 112(g) Technical Background Document;
- EPA Documentation of De Minimis Emission Rates Proposed 40 CFR Part 63, Subpart B Background Document;
- EPA Health Effects Notebook for Hazardous Air Pollutants (HAPfacts);
- EPA Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons.
- Agency for Toxic Substances and Disease Registry Minimal Risk Levels (MRLs);
- California Environmental Protection Agency Non-cancer Reference Exposure Levels (REL), Reference Doses (RfDs), Cancer Slope Factors (CSFs), and Unit Risks (URs);
- EPA Hazardous Air Pollutants: Profiles of Non-cancer Toxicity from Inhalation Exposures (HAPs Profiles);
- Agency for Toxic Substances and Disease Registry Toxicological Profiles;
- International Agency for Research on Cancer (IARC), weights of evidence (WOE);
- U.S. National Library of Medicine, Hazardous Substances Data Bank; and

These data sources were selected based on the applicability of the toxicological information to the needs of the Cumulative Exposure Study, the number of chemicals for which there was available information, and the reliability and age of the data.

The following sections provide a review of each data source and the data it contributed.

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Integrated Risk Information System (IRIS)

The *Integrated Risk Information System* (IRIS) consolidates EPA's human health risk and regulatory information for specific chemicals in an electronic database.⁶ This database provides consistent, up-to-date toxicity information for EPA staff across all agency programs.

The IRIS database contains toxicological information that has been verified by the EPA's Reference Dose/Reference Concentration (RfD/RfC) Work Group, or EPA's Carcinogen Risk Assessment Verification Endeavor (CRAVE) Work Group. These work groups review the toxicity data in a process that leads to agency-wide consensus on toxicity values.

IRIS contains toxicological information on non-cancer and cancer health effects. Specific data elements include chronic reference concentrations (RfC) for inhalation exposures, chronic reference doses (RfD) for oral exposures, cancer slope factors (CSF) for oral exposures, and unit risk (UR) values for inhalation exposures, for all pollutants for which such values have been verified by the EPA work groups. IRIS does not contain information on acute health effects. Exhibit 3-20 provides a list of toxicity benchmark and potency values used in developing the Cumulative Exposure Toxicity Database. The critical health effects associated with RfDs and RfCs are included, as are the types of cancer associated with CSFs and URs.

EPA updates IRIS data monthly. The database uses IRIS data current through January 1, 1998.

Exhibit 3-20

TOXICITY DATA ELEMENTS IN IRIS INCLUDED IN THE DATABASE

Chronic Reference Concentration (RfC) (mg/cu m)

Confidence level in the RfC (high, medium, low)

Critical effect associated with RfC

Chronic Reference Dose (RfD) (mg/kg/day)

Confidence level in the RfD (high, medium, low)

Critical effect associated with RfD

Oral Cancer Slope Factor (O_CSF) (mg/kg/day)⁻¹

Type of cancer associated with exposure through oral ingestion

Inhalation Unit Risk Value (ISF UR) (µg/cu m)⁻¹

Type of cancer associated with exposure through inhalation

EPA Carcinogenic Weight of Evidence category

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⁶ U.S. Environmental Protection Agency, *Integrated Risk Information System, Introduction to IRIS*, June 1993.

Health Effects Assessment Summary Tables

EPA's *Health Effects Assessment Summary Tables* (HEAST), prepared by EPA's National Center for Environmental Assessment, consolidates human health risk information for chemicals of interest to EPA's CERCLA and RCRA programs.⁷ Information contained in HEAST is gathered from documents developed by EPA offices for specific chemicals.

As shown in Exhibit 3-21, HEAST contains four types of data that are useful for the Cumulative Exposure database:

- Chronic and subchronic non-cancer toxicity values (oral RfDs and inhalation RfCs) developed using the same methods as the EPA RfD/RfC Work Group;
- Chronic and subchronic non-cancer toxicity values (oral RfDs and inhalation RfCs) contained in EPA documents, and developed using methods that may be different than those of the EPA RfD/RfC Work Group;
- Cancer slope factors (CSFs) and unit risks (URs) developed using the same methods as the CRAVE Work Group; and
- Radionuclide cancer slope factors provided by the Office of Radiation Programs.

HEAST does not contain information on health effects other than the critical effects associated with the derivation of the toxicity values. HEAST also does not contain information on acute health effects.

Unless otherwise stated, EPA considers the toxicity values in HEAST to be provisional since neither the RfD/RfC Work Group nor the CRAVE Work Group has reviewed the values and their derivation. Although the HEAST data do not have the agency-wide consensus of the IRIS data, the information contained in HEAST represents current toxicity data generated by EPA.

The most recent version of the HEAST tables was developed in 1995. The HEAST data used in the database was obtained from the 1998 first quarter version of Smarttox.⁸ Exhibit 3-21 lists the HEAST toxicological information used in the database. Smarttox gives preference to

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⁷ U.S. Environmental Protection Agency, *Health Effects Assessment Summary Tables*, 1997.

⁸ Pioneer Systems Development, *Smarttox Toxicity Value Lookup Table*, January, 1998. Smarttox is a toxicity value lookup table that combines chronic and subchronic toxicity values from both IRIS and HEAST into one database system.

IRIS toxicity values, with HEAST values used only in cases where IRIS values are not available. For each toxicity value in Smarttox, the source of the value is presented, as well as information on whether or not the value was derived using the RfD/RfC Work Group method.

Exhibit 3-21

TOXICITY DATA ELEMENTS IN HEAST INCLUDED IN THE DATABASE

Chronic Reference Concentration (RfC) (mg/cu m)

Health effect associated with the RfC

Chronic Reference Dose (RfD) (mg/kg/day)

Health effect associated with the RfD

Subchronic Reference Concentration (Sub-RfC)

Health effect associated with Sub-RfC

Subchronic Reference Dose (Sub-RfD)

Health effect associated with Sub-RfD

Oral Cancer Slope Factor (O_CSF) (mg/kg/day)⁻¹

Type of cancer associated with exposure through oral ingestion

Inhalation Unit Risk (ISF_UR) (µg/cu m) ⁻¹

Type of cancer associated with exposure through inhalation

Levels of Concern for SARA Title III Extremely Hazardous Substances

EPA has established Levels of Concern (LOC) for chemicals on the Superfund Amendments and Reauthorization Act (SARA) Title III Section 302 list of "extremely hazardous substances." The LOC is defined as "the concentration of an extremely hazardous substance in air above which there may be serious irreversible health effects or death as a result of a single exposure for a relatively short period of time." EPA bases its estimate of this value on one-tenth of the "Immediately Dangerous to Life and Health" (IDLH) values generated by NIOSH. If IDLH values were not available, EPA used other sources with acute toxicity information, such as threshold limit values established by the American Conference of Governmental Industrial Hygienists and guidelines developed by the National Research Council of the National Academy of Science.

LOCs provide acute toxicity benchmarks for air pollutants. As a result, LOCs are only applicable to inhalation exposures and cannot be used to evaluate exposures through oral ingestion. There are other limitations associated with the use of LOCs to evaluate human health effects associated with acute exposure to pollutants in EPA's Cumulative Exposure Study. First, LOCs do not provide information on the maximum duration of exposure at the LOC that would

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⁹ U.S. Environmental Protection Agency, *Technical Guidance for Hazards Analysis*, *Emergency Planning for Extremely Hazardous Substances*, December 1987.

be considered safe, nor do they provide information on the associated acute health effects. Second, the safety factor of 10 used to derive LOCs from IDLHs may not be adequate due to concern about the scientific peer review of the rationale and supporting data for each LOC. ¹⁰ Finally, many of the IDLH values, from which LOC values are derived, are based on animal data, and may not protect against all human health effects.

The database uses LOC values from two sources -- the 1987 technical guidance document for emergency planning for Extremely Hazardous Substances (EHS)¹¹ and the Clean Air Act Amendments Section 112(g) Technical Background Document (described below)¹². The LOC values contained in the Section 112(g) document are based on the 1987 SARA Section 302 technical support document, but some of them have been updated by EPA's Office of Solid Waste and Emergency Response. In cases where LOC values are available from both sources, only the value from the Section 112(g) document is included in the database.

Clean Air Act Section 112(g) Technical Background Document

EPA's Clean Air Act Section 112(g) *Technical Background Document* describes the method developed by the EPA to rank air pollutants with respect to human health hazard. ¹³ This method was developed as part of the 1990 Clean Air Act Amendments (CAAA) to determine the relative hazard posed by hazardous air pollutants (HAPs) for the purpose of determining allowable offsets.

As part of the Section 112(g) hazard ranking, EPA presents toxicological information for each of the HAPs. This information was gathered from secondary sources. The Cumulative Exposure Toxicity Database contains LOC values and weight of evidence classifications for carcinogenicity from the Section 112(g) document.

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¹⁰ Caldwell, Jane C., Tracey J. Woodruff, Rachel Morello-Frosch, and Daniel A. Axelrad, "Application of Health Information to Hazardous Air Pollutants Modeled in EPA's Cumulative Exposure Project," *Toxicology and Industrial Health*, vol. 14, p. 429-54, 1998.

¹¹ U.S. Environmental Protection Agency, *Technical Guidance for Hazards Analysis, Emergency Planning for Extremely Hazardous Substances*, December 1987.

¹² U.S. Environmental Protection Agency, *Technical Background Document to Support Rulemaking Pursuant to the Clean Air Act-Section 112(g), Ranking of Pollutants with Respect to Hazard to Human Health*, EPA-450/3-92-010, Office of Air Quality Planning and Standards, February, 1994.

¹³ Ibid.

Documentation of De Minimis Emissions Rates

Clean Air Act Section 112(g) requires control technology determinations for changes to plant sites that cause emissions increases above *de minimis* levels. EPA's *Documentation of De minimis Emissions Rates*, provides information about the proposed *de minimis* levels and their basis. The report contains carcinogenic data (i.e., weight of evidence classifications, cancer slope factors, and inhalation unit risks) for hazardous air pollutants. These data were aggregated from numerous EPA sources, including IRIS, Health and Environmental Assessments (HEA), Health Assessment Documentation (HAD), the Health Effect and Environmental Profile (HEEP), the Offices of Research and Development (ORD), and the Risk Assessment Forum (RAF) report.

Cancer data reported in EPA's *Documentation of DeMinimis Emission Rates* and derived from EPA sources other than IRIS and HEAST are included in the database.

Health Effects Notebook for Hazardous Air Pollutants

The *Health Effects Notebook for Hazardous Air Pollutants* (HAPfacts) contains chemical fact sheets of toxicity data for each of the Hazardous Air Pollutants specified in the Clean Air Act Amendments of 1990.¹⁵ EPA's Air Risk Information Support Center developed these fact sheets as a tool for quick access to toxicological information and reference sources, and they were updated most recently in December 1994.

Each HAPfacts chemical fact sheet provides descriptions of health effects, including reproductive and developmental effects, associated with exposure to a pollutant. Toxicological information presented in the fact sheets are for both inhalation and oral routes of exposure. These qualitative data were used to develop the Qualitative Health Effects Table in the Cumulative Exposure Toxicity Database.

HAPfacts also contains both verified and provisional RfDs and RfCs (including specific values for acute and chronic effects) and cancer slope factors. Since many of the data sources used to develop the worksheets are the same as those discussed above (e.g., IRIS, HEAST), these quantitative values were not put into the database to avoid duplication.

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¹⁴ U.S. Environmental Protection Agency, *Documentation of De minimis Emission Rates* - *Proposed 40 CFR Part 63, Subpart B Background Document*, EPA-453/R-93-035, Office of Air Quality Planning and Standards, February 1994.

¹⁵ U.S. Environmental Protection Agency, *Health Effects Notebook for Hazardous Air Pollutants*, December 1994.

Agency for Toxic Substances and Disease Registry Minimal Risk Levels (MRLs)

The Agency for Toxic Substances and Disease Registry (ATSDR) initially developed Minimal Risk Levels (MRLs) in response to a mandate specified in the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) requiring ATSDR, in conjunction with EPA, to develop significant human exposure levels for hazardous substances in the environment. ATSDR's MRLs represent the maximum exposure levels that would not lead to the development of non-cancer health effects in humans, based on acute, subchronic and chronic exposures. ¹⁶

ATSDR develops these MRLs based on no observed adverse effect levels (NOAELs) for the most sensitive populations, similar to the process used to derive EPA's RfDs. All MRLs developed by ATSDR are reviewed by four separate groups: the Health Effects/MRL Work Group within the Division of Toxicology; an expert panel of external peer reviewers; the agencywide MRL Work Group, with participation from other federal agencies, including EPA; and the public, through the toxicological profile public comment period.

ATSDR provides MRLs for acute, chronic, and subchronic exposures. Additionally, for each MRL, ATSDR provides information on the route of exposure (oral or inhalation) and the adverse health effect associated with the value. Exhibit 3-22 lists the MRL information provided by ATSDR that is included in the Cumulative Exposure Toxicity Database.

Exhibit 3-22

DATA ELEMENTS AVAILABLE FROM ATSDR (MRLs) INCLUDED IN THE DATABASE

MRL associated with chronic inhalation exposures (mg/cu m), and the associated health effect

MRL associated with chronic oral exposures (mg/kg/day), and the associated health effect

MRL associated with subchronic inhalation exposures (mg/cu m), and the associated health effect

MRL associated with subchronic oral exposures (mg/kg/day), and the associated health effect

MRL associated with acute inhalation exposures (mg/cu m), and the associated health effect

MRL associated with acute oral exposures (mg/kg/day), and the associated health effect

MRLs are readily available from the ATSDR internet site. The MRL data included in the database was downloaded from the internet site in February 1998.

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Agency for Toxic Substances and Disease Registry, *Minimal Risk Levels for Hazardous Substances*, December 1997, http://atsdr1.atsdr.cde.gov:8080/hrls.html, obtained February 1998.

California Environmental Protection Agency Non-cancer and Cancer Toxicity Values

The California Environmental Protection Agency (Cal EPA) has established toxicity values for both non-cancer and cancer health effects for use in chemical risk assessment.¹⁷ The database contains two types of Cal EPA non-cancer toxicity values -- reference doses (RfDs) and reference exposure levels (RELs). Cal EPA developed RfDs for determining drinking water standards and action levels that are maintained by the California Office of Environmental Health Hazard Assessment (Cal OEHHA). It established RELs for the Air Toxics "Hot Spots" program.

Chronic RELs were developed by the California Air Pollution Control Officers' Association (CAPCOA) with consultation from Cal OEHHA, and are based on values previously established in readily available sources. Sources used include EPA databases (e.g., IRIS, HEAST), the American Conference of Governmental Industrial Hygienists' Threshold Limit Values, and studies conducted by Cal EPA. In addition, CAPCOA developed acute RELs, which are listed in the CAPCOA Risk Assessment Guidelines.¹⁸

The Cumulative Exposure Toxicity Database also contains Cal EPA cancer potency values. These values include cancer slope factors for oral exposures, as well as unit risk values for exposures to contaminants via the inhalation exposure pathway.¹⁹ These cancer potency values were approved or developed by Cal EPA's Office of Environmental Health Hazard Assessment, Department of Pesticide Regulation, and Department of Toxic Substances Control.

Hazardous Air Pollutants: Profiles of Non-cancer <u>Toxicity from Inhalation Exposures (HAPs Profiles)</u>²⁰

HAPs Profiles provide inhalation data on $LC_{50}s$, NOAELs, and LOAELs for chemicals listed as Hazardous Air Pollutants (HAPs) under the 1990 Clean Air Act Amendments. EPA's Office of Health Research identified and compiled these data in order to identify data gaps and

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¹⁷ Risk Assessment Advisory Committee, *A Review of the California Environmental Protection Agency's Risk Assessment Practices, Policies, and Guidelines*, California Environmental Protection Agency, 1996.

¹⁸ California Air Pollution Control Officers' Association, *Air Toxics "Hot Spots" Program Risk Assessment Guidelines*, October 1993.

¹⁹ California Environmental Protection Agency, Standards and Criteria Work Group, *California Potency Factors: Update*, April 1, 1996, obtained from http://www.calepa.cahwnet.gov/oehha/docs/covrltrb.htm, April 1998.

²⁰ U.S. Environmental Protection Agency, *Hazardous Air Pollutants: Profiles of Noncancer Toxicity from Inhalation Exposures*, 1993.

research priorities and to assist federal, state and local governments in evaluating the health risks posed by these chemicals. The Cumulative Exposure Toxicity Database incorporates HAPs Profiles' LOAEL, NOAEL, and LC₅₀ data into its Inhalation LOAEL, NOAEL, & LC₅₀ Table.

HAPs Profiles aggregate data from multiple secondary sources. These include the *Integrated Risk Information System* (IRIS), EPA's *Health Assessment Documents* (HAD) and *Drinking Water Criteria Documents* (DWCD), the *Health Effects Assessment Summary Tables* (HEAST), the Agency for Substances and Disease Registry's (ATSDR) *Supplemental Tables*, and the National Library of Medicine's Hazardous Substances Data Bank (HSDB). EPA reviewed IRIS for every HAP, and developed a preferential hierarchy for compiling data from the other sources. According to that hierarchy, HAD, DWCD, ATSDR's *Supplemental Tables*, HSDB, and HEAST were utilized in that order. For example, ATSDR's *Supplemental Tables* were used only for chemicals lacking data in HAD or DWCD, and HSDB was used only when the ATSDR source also lacked data.

Some of the HAPs Profiles sources listed above provide information only about the critical health effects used to determine standard benchmark values such as RfDs, while others contain data on multiple health endpoints. Most of these data are for animals and have not been adjusted for human exposure.

Each study listed in HAPs Profiles contains numerical references to notes that provide information about the studies on which the toxicity values are based and allow the user to judge the reliability and quality of the data. HAPs Profiles' data and associated notes were reviewed prior to inclusion in the database. Records for which the notes clearly indicated poor quality or inappropriate data for the purposes of the Cumulative Exposure Toxicity Database were not entered. In addition, some HAPs Profiles data were not included in the database for the following reasons.

- Only one dose was tested.
- The information was obviously anecdotal. (For example, several records described the health effects reported as a result of a teenager's recreational abuse of a chemical.)
- The test population was exposed concurrently to other compounds, and those chemicals composed more than two percent of the chemical mixture.
- The reported exposure concentrations were estimated and may not have been representative of actual exposures.
- The exposure concentrations were unknown.
- The test population was exposed via exposure routes other than inhalation.

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• The toxicity data was not one of the three types included in the Inhalation LOAEL, NOAEL, and LC₅₀ table. For example, some data were provided for RD₅₀s, which represent concentrations at which 50 percent of sample populations experience respiratory health effects.

Despite these quality control measures, not all of the HAPs Profiles' data included in the database may be adequate for each user's specific needs. Therefore, database users may wish to consult the notes in the HAPs Profiles document (as referenced in the *Notes* field in the database) to ensure the adequacy of the data.

Agency for Toxic Substances and Disease Registry Toxicological Profiles

Section 104(i)(3) of the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), as amended, directs the Agency for Toxic Substances and Disease Registry (ATSDR) to prepare toxicological profiles for compounds on the Superfund list of hazardous substances that are commonly found at hazardous waste sites on the National Priority List. The revised list of the 275 most hazardous substances was published in the Federal Register on October 28, 1992 (57 FR 48801).

Each profile includes an examination, summary, and interpretation of the available toxicological information and epidemiological studies on a hazardous substance in order to ascertain the levels of significant human exposure for the substance and the associated health effects. Each profile identifies and reviews the key peer-reviewed literature that describes a hazardous substance's toxicological properties. The information in the Toxicological Profiles has been reviewed extensively by scientists from ATSDR, the Centers for Disease Control and Prevention (CDC), and other federal agencies, as well as by a panel of peer reviewers from outside the government.

The Cumulative Exposure Toxicity Database uses LOAEL, NOAEL, LD_{50} and LC_{50} data reported in tables from the Toxicological Profiles that summarize peer-reviewed primary toxicological and epidemiological literature.²¹ These tables were primarily used to obtain data relating to the oral route of exposure. They were also used to provide inhalation LOAEL, NOAEL, and LC_{50} data for chemicals without such data in HAPs Profiles.

International Agency for Research on Cancer (IARC)

IARC was established in 1965 by the World Health Organization to coordinate and conduct research on the causes of human cancer and to develop strategies for controlling cancer. IARC has evaluated the carcinogenic risks of more than 800 agents (e.g., chemicals, chemical

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²¹ Agency for Toxic Substances and Disease Registry, *Toxicological Profiles on CD-ROM*, CRC Press, Inc., 1997.

groups, occupational exposures, cultural habits, etc.). Based on its evaluations, IARC assigns each agent a weight of evidence category for carcinogenicity in humans. These weight of evidence categories, obtained from IARC's internet site, are incorporated into the Cancer Health Effects Table of the Cumulative Exposure Toxicity Database.²²

Hazardous Substances Data Bank (HSDB)

The U.S. National Library of Medicine and the National Institute of Health have developed a computerized system (TOXNET) that provides on-line access to a variety of data sources containing information on toxicology. One such data source, HSDB, contains extensive listings of chemical synonyms as part of its chemical profiles. This information was used to develop the Synonyms Table in the Cumulative Exposure Toxicity Database. HSDB provided more than 5,000 synonyms for the 344 chemicals listed in the General Information Table of the database.

Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons²³

This 1993 EPA report provides estimates of the relative cancer potencies, or toxic equivalency factors (TEFs), for several polycyclic aromatic hydrocarbons (PAHs). The estimates use benzo(a)pyrene as a reference compound. For example, EPA estimated that benzo(a)anthracene is one tenth as potent as benzo(a)pyrene. The Toxic Equivalency Factors Table in the database contains these TEF data, and several of the database searches use the data to estimate oral slope factors when other toxicity benchmarks are not available.

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²² International Agency for Research on Cancer, "Overall Evaluations of Carcinogenicity to Humans," obtained from http://www.iarc.fr/monoeval/crthall.htm, November 21, 1997.

²³ U.S. Environmental Protection Agency, *Provisional Guidance for Quantitative Risk Assessment of Polycyclic Aromatic Hydrocarbons*, EPA/600/R-93-089, July 1993.

LIST OF CHEMICALS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

LIST OF CHEMICALS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

1	<u>Chemical Name</u> Acenaphthene	CAS Number* 83-32-9
2	Acephate	30560-19-1
3	Acetaldehyde	75-07-0
4	Acetamide	60-35-5
5	Acetonitrile	75-05-8
6	Acetophenone	98-86-2
7	Acrolein	107-02-8
8	Acrylamide	79-06-1
9	Acrylic acid	79-10-7
10	Acrylonitrile	107-13-1
11	Alachlor	15972-60-8
12	Aldicarb	116-06-3
13	Aldrin	309-00-2
14	Allyl chloride	107-05-1
15	Aminobiphenyl, 4-	92-67-1
16	Aniline	62-53-3
17	Anisidine	90-04-0
18	Anthracene	120-12-7
19	Antimony and Compounds	7440-36-0
20	Antimony and Compounds Antimony pentafluoride	7783-70-2
21	Antimony pentariadride Antimony pentariadride	1314-60-9
22	Antimony potassium tartrate	304-61-0
23	Antimony potassium tartate Antimony tetroxide	1332-81-6
24	Antimony trioxide	1309-64-4
25	Antimony trioxide Antimony trisulfide	1345-04-6
26	Aroclor 1016	12674-11-2
27	Aroclor 1221	11104-28-2
28	Aroclor 1221 Aroclor 1242	53469-21-9
29	Aroclor 1248	12672-29-6
30	Aroclor 1254	11097-69-1
31	Aroclor 1260	11096-82-5
32	Arsenic and Compounds	7440-38-2
33	Arsenic chloride	7784-34-1
34	Arsenic oxide	1327-53-3
35	Arsenic pentoxide	1303-28-2
36	Arsine	7784-42-1
37	Asbestos	1332-21-4
38	Atrazine	1912-24-9
39	Azinphos-methyl	86-50-0
40	Bendiocarb	22781-23-3
41	Benzene	71-43-2
42	Benzo(a)anthracene	56-55-3
43	Benzo(a)pyrene	50-32-8
44	Benzo(b)fluoranthene	205-99-2
45	Benzo(g,h,i)perylene	191-24-2
46	Benzo(k)fluoranthene	207-08-9
47	Benzotrichloride	98-07-7
48	Benzyl chloride	100-44-7
.5	20112/101100	100 11 /

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LIST OF CHEMICALS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

	Chemical Name	CAS Number*
49	Beryl ore	1302-52-9
50	Beryllium and Compounds	7440-41-7
51	Beryllium carbonate	66104-24-3
52	Beryllium chloride	7787-47-5
53	Beryllium fluoride	7787-49-7
54	Beryllium hydrogen phosphate	13598-15-7
55	Beryllium nitrate	13597-99-4
56	Beryllium orthophosphate	35089-00-0
57	Beryllium oxide	1304-56-9
58	Beryllium sulfate	13510-49-1
59	Biphenyl	92-52-4
60	Bis(2-ethylhexyl)phthalate	117-81-7
61	Bis(chloromethyl)ether	542-88-1
62	Bromodichloromethane	75-27-4
63	Bromoform	75-25-2
64	Butadiene, 1,3-	106-99-0
65	Cadmium and Compounds	7440-43-9
66	Cadmium oxide	1306-19-0
67	Cadmium stearate	2223-93-0
68	Calcium cyanamide	156-62-7
69	Calcium cyanide	592-01-8
70	Caprolactam	105-60-2
71	Captan	133-06-2
72	Carbaryl	63-25-2
73	Carbon disulfide	75-15-0
74	Carbon monoxide	630-08-0
75	Carbon tetrachloride	56-23-5
76	Carbonyl sulfide	463-58-1
77	Catechol	120-80-9
78	Chloramben	133-90-4
79	Chlordane	57-74-9
80	Chlorinated dibenzo-p-dioxins (as 2,3,7,8-equivalents)	dioxins
81	Chlorinated dibenzofurans (as 2,3,7,8-equivalents)	furans
82	Chlorine	7782-50-5
83	Chlorine cyanide	506-77-4
84	Chloroacetic acid	79-11-8
85	Chlorobenzene	108-90-7
86	Chloroform	67-66-3
87	Chloromethyl methyl ether	107-30-2
88	Chloroprene	126-99-8
89	Chloropropham	101-21-3
90	Chlorothalonil	1897-45-6
91	Chlorpyrifos	2921-88-2
92	Chromium (III) Compounds	16065-83-1
93	Chromium (VI) Compounds	18540-29-9
94	Chromium and Compounds	7440-47-3
95	Chromium chloride	10025-73-7
96	Chrysene	218-01-9

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LIST OF CHEMICALS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

0.7	Chemical Name	CAS Number*
97	Cobalt acetate	71-48-7
98	Cobalt and Compounds	7440-48-4
99	Cobalt bromide	7789-43-7
100	Cobalt carbonate	513-79-1
101	Cobalt carbonyl	10210-68-1
102	Cobalt chloride	7646-79-9
103	Cobalt fluoride	10026-17-2
104	Cobalt nitrate	Co Nitrate
105	Cobalt oxides (mixed)	COBOXIDES
106	Cobalt phosphate	13455-36-2
107	Cobalt sulfate	10124-43-3
108	Copper cyanide	544-92-3
109	Cresol, m-	108-39-4
110	Cresol, o-	95-48-7
111	Cresol, p-	106-44-5
112	Cresols (mixed)	1319-77-3
113	Cumene	98-82-8
114	Cyanazine	21725-46-2
115	Cyanide and Compounds	57-12-5
116	Cyanogen	460-19-5
117	Cyanogen bromide	506-68-3
118	Cyanogen iodide	506-78-5
119	Cyanophos	2636-26-2
120	Cyanuric fluoride	675-14-9
121	D, salts and esters, 2,4-	94-75-7
122	DDD	72-54-8
123	DDE	72-55-9
124	DDT	50-29-3
125	Diazinon	333-41-5
126	Dibenz(a,h)anthracene	53-70-3
127	Dibromochloromethane	124-48-1
128	Dibutylphthalate	84-74-2
129	Dichlorobenzene, p-	106-46-7
130	Dichlorobenzidine, 3,3'-	91-94-1
131	Dichloroethyl ether	111-44-4
132	Dichloropropene, 1,3-	542-75-6
133	Dichlorvos	62-73-7
134	Dieldrin	60-57-1
135	Diethanolamine	111-42-2
136	Diethylaniline, N,N-	91-66-7
137	Diethyl sulfate	64-67-5
138	Diethyl/dimethylaniline, N,N-	Dialks
139	Diethylene glycol monobutyl ether	112-34-5
140	Diethylene glycol monoethyl ether	111-90-0
141	Dimethoxybenzidine, 3,3'-	119-90-4
142	Dimethylaniline, N,N-	121-69-7
143	Dimethyl anthracene, 9,10-	781-43-1
144	Dimethyl formamide	68-12-2

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LIST OF CHEMICALS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

	Chamical Name	CAC Name book
145	Chemical Name	<u>CAS Number*</u> 131-11-3
	Dimethyl phthalate	
146	Dimethyl sulfate	77-78-1
147	Dimethylbenz(a)anthracene, 7,12-	57-97-6 57-14-7
148	Dimethylhydrazine, 1,1-	57-14-7 524-52-1
149	Dinitro-o-cresol, 4,6-	534-52-1
150	Dinitrophenol, 2,4-	51-28-5
151	Dinitrotoluene, 2,4-	121-14-2
152	Dinitrotoluene, 2,4/2,6-	25321-14-6
153	Dioxane, 1,4-	123-91-1
154	Diphenylamine	122-39-4
155	Endosulfans	115-29-7
156	Epichlorohydrin	106-89-8
157	Epoxybutane, 1,2-	106-88-7
158	Ethyl acrylate	140-88-5
159	Ethyl benzene	100-41-4
160	Ethyl carbamate	51-79-6
161	Ethyl chloride	75-00-3
162	Ethylene dibromide	106-93-4
163	Ethylene dichloride	107-06-2
164	Ethylene glycol	107-21-1
165	Ethylene glycol butyl ether	111-76-2
166	Ethylene glycol ethyl ether	110-80-5
167	Ethylene glycol ethyl ether acetate	111-15-9
168	Ethylene glycol methyl ether	109-86-4
169	Ethylene glycol methyl ether acetate	110-49-6
170	Ethylene oxide	75-21-8
171	Ethylene thiourea	96-45-7
172	Ethylidene dichloride	75-34-3
173	Ethylmercuric phosphate	2440-45-1
174	Fluomine	62207-76-5
175	Fluoranthene	206-44-0
176	Fluorene	86-73-7
177	Formaldehyde	50-00-0
178	Glycol ethers	Glyc Eth
179	Heptachlor	76-44-8
180	Hexachlorobenzene	118-74-1
181	Hexachlorobutadiene	87-68-3
182	Hexachlorocyclopentadiene	77-47-4
183	Hexachlorodibenzo-p-dioxin, mixture	19408-74-3
184	Hexachloroethane	67-72-1
185	Hexane	110-54-3
186	Hydrazine	302-01-2
187	Hydrochloric acid	7647-01-0
188	Hydrofluoric acid	7664-39-3
189	Hydrogen cyanide	74-90-8
190	Hydrogen selenide	7783-07-5
191	Hydroquinone	123-31-9
192	Imazalil	35554-44-0
1/4	mazam	3333 7-44- U

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LIST OF CHEMICALS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

	Chemical Name	CAS Number*
193	Indeno(1,2,3-cd)pyrene	193-39-5
194	Iprodione	36734-19-7
195	Lead acetate	301-04-2
196	Lead and Compounds	7439-92-1
197	Lead chloride	7758-95-4
198	Lead nitrate	10099-74-8
199	Lead subacetate	1335-32-6
200	Lindane	58-89-9
201	Malathion	121-75-5
202	Maleic anhydride	108-31-6
203	Manganese acetate	638-38-0
204	Manganese and Compounds	7439-96-5
205	Manganese chloride	7773-01-5
206	Manganese dioxide	1313-13-9
207	Manganese oxide	1317-35-7
208	Manganese salts and oxides	MNSALTOXIDE
209	Manganese sulfate	7785-87-7
210	Manganese tricarbonyl methylcyclopentadienyl	12108-13-3
211	Mercuric acetate	1600-27-7
212	Mercuric chloride	7487-94-7
213	Mercuric nitrate	10045-94-0
214	Mercuric oxide	21908-53-2
215	Mercuric sulfide	1134-48-5
216	Mercury and Compounds	7439-97-6
217	Methamidophos	10265-92-6
218	Methanol	67-56-1
219	Methoxychlor	72-43-5
220	Methoxyethylmercuric acetate	151-38-2
221	Methyl bromide	74-83-9
222	Methyl chloride	74-87-3
223	Methyl chloroform	71-55-6
224	Methyl ethyl ketone	78-93-3
225	Methyl hydrazine	60-34-4
226	Methyl iodide	74-88-4
227	Methyl isobutyl ketone	108-10-1
228	Methyl isocyanate	624-83-9
229	Methyl mercury	22967-92-6
230	Methyl methacrylate	80-62-6
231	Methyl tert-butyl ether	1634-04-4
232	Methylene bis(2-chloroaniline), 4,4'-	101-14-4
233	Methylene chloride	75-09-2
234	Methylene diphenyl diisocyanate	101-68-8
235	Methylenedianiline, 4,4'-	101-77-9
236	Methylmercuric chloride	115-09-3
237	Methylmercuric dicyanamide	502-39-6
238	Naphthalene	91-20-3
239	Nickel acetate	373-02-4
240	Nickel and Compounds	7440-02-0

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LIST OF CHEMICALS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

2.11	Chemical Name	CAS Number*
241	Nickel carbonyl	13463-39-3
242	Nickel chloride	7718-54-9
243	Nickel nitrate	13138-45-9
244	Nickel oxide	1313-99-1
245	Nickel subsulfide	12035-72-2
246	Nickel sulfate	7786-81-4
247	Nicotine	54-11-5
248	Nitrobenzene	98-95-3
249	Nitrophenol, 4-	100-02-7
250	Nitropropane, 2-	79-46-9
251	Nitrosodimethylamine	62-75-9
252	Parathion	56-38-2
253	Particulate matter	Part Matter
254	Pentachlorodibenzofuran, 2,3,4,7,8-	57117-31-4
255	Pentachloronitrobenzene	82-68-8
256	Pentachlorophenol	87-86-5
257	Permethrin	52645-53-1
258	Phenanthrene	85-01-8
259	Phenol	108-95-2
260	Phenylenediamine, p-	106-50-3
261	Phenylmercuric acetate	62-38-4
262	Phenylphenol, o-	90-43-7
263	Phosgene	75-44-5
264	Phosphorus	7723-14-0
265	Phthalic anhydride	85-44-9
266	Plutonium and Compounds	7440-07-5
267	Plutonium nitrate	14913-29-2
268	Plutonium oxide	Pu Oxide
269	Polychlorinated biphenyls	1336-36-3
270	Polycyclic aromatic hydrocarbons	PAHs
271	Polycyclic Organic Matter	POM
272	Potassium cyanide	151-50-8
273	Potassium selenate	7790-59-2
274	Potassium silver cyanide	506-61-6
275	Potassium thiocyanate	333-20-0
276	Propionaldehyde	123-38-6
277	Propoxur	114-26-1
278	Propylene dichloride	78-87-5
279	Propylene glycol monoethyl ether	52125-53-8
280	Propylene glycol monomethyl ether	107-98-2
281	Propylene glycol, allyl ether	1331-17-5
282	Propylene oxide	75-56-9
283	Propyleneimine, 1,2-	75-55-8
284	Pyrene	129-00-0
285	Quinoline	91-22-5
286	Quinone	106-51-4
287	Radionuclides	Radio
288	Radium	7440-14-4

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Appendix A

LIST OF CHEMICALS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

	Chemical Name	CAS Number*
289	Radon	10043-92-2
290	Selenic acid	7783-08-6
291	Selenious acid	7783-00-8
292	Selenium and Compounds	7782-49-2
293	Selenium dioxide	7446-08-4
294	Selenium disulfide	7488-56-4
295	Selenium oxychloride	7791-23-3
296	Selenium sulfide	7446-34-6
297	Silver cyanide	506-64-9
298	Simazine	122-34-9
299	Sodium cyanide	143-33-9
300	Sodium selenate	13410-01-0
301	Sodium selenide	1313-85-5
302	Sodium selenite	10102-18-8
303	Styrene	100-42-5
304	Styrene oxide	96-09-3
305	Tetrachlorodibenzo-p-dioxin, 2,3,7,8-	1746-01-6
306	Tetrachloroethane, 1,1,2,2-	79-34-5
307	Tetrachloroethene	127-18-4
308	Tetraethyl lead	78-00-2
309	Tetramethyl lead	75-74-1
310	Thiabendazole	148-79-8
311	Thiocyanic acid, 2-(Benzothiazolylthio) methyl ester	21564-17-0
312	Titanium tetrachloride	7550-45-0
313	Toluene	108-88-3
314	Toluene diamine, 2,4-	95-80-7
315	Toluene diisocyanate mixture (TDI), 2,4/2,6-	26471-62-5
316	Toluene diisocyanate, 2,4-	584-84-9
317	Toluidine, o-	95-53-4
318	Toxaphene	8001-35-2
319	Trichlorobenzene, 1,2,4-	120-82-1
320	Trichloroethane, 1,1,2-	79-00-5
321	Trichloroethylene	79-01-6
322	Trichlorophenol, 2,4,6-	88-06-2
323	Trifluralin	1582-09-8
324	Trimethylpentane, 2,2,4-	540-84-1
325	Uranium and Compounds	7440-61-1
326	Uranium dioxide	1334-57-6
327	Uranium hexafluoride	7783-81-5
328	Uranium peroxide	19525-15-6
329	Uranium tetrachloride	10026-10-5
330	Uranium tetrafluoride	10049-14-6
331	Uranium, soluble salts	URANSOLS
332	Uranyl acetate dihydrate	541-09-3
333	Uranyl fluoride	13536-84-0
334	Uranyl nitrate hexahydrate	13520-83-7
335	Vinyl acetate	108-05-4
336	Vinyl bromide	593-60-2

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Appendix A

LIST OF CHEMICALS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

	Chemical Name	CAS Number*
337	Vinyl chloride	75-01-4
338	Vinylidene chloride	75-35-4
339	Xylene, m-	108-38-3
340	Xylene, o-	95-47-6
341	Xylene, p-	106-42-3
342	Xylenes (mixed)	1330-20-7
343	Zinc beryllium silicate	39413-47-3
344	Zinc cyanide	557-21-1

^{*} Chemicals or chemical groups lacking CAS numbers or for which CAS numbers could not be identified have been assigned unique identifiers in the database.

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LIST OF CHEMICAL GROUPS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

LIST OF CHEMICAL GROUPS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

The list of chemicals in the Cumulative Exposure Database (Appendix A) was developed based on the Cumulative Exposure Study. The database includes the full list of individual chemicals that were analyzed in the study. In addition to these individual chemicals, the study analyzed groups of chemicals such as mercury compounds or polycyclic organic matter. The database includes additional individual chemicals from the sources reviewed that belong to one of the chemical groups that were analyzed. For example, neither mercuric acetate nor methyl mercury was evaluated in the Cumulative Exposure Study, but both are in the database because mercury compounds were evaluated as group. Exhibit B-1 lists the subset of chemicals in the database that belong to chemical groups. The exhibit organizes the chemicals alphabetically by group.

The list of compounds for each group usually contains one or more names in italics. These are the generic names used for data related to an entire group or subgroup of chemicals. For example, "Cresols (mixed)" is italicized in the exhibit, indicating that any data that apply to cresols in general, or to a mixture of cresols, are listed in the database under the name "Cresols (mixed)." In the case of metal and radionuclide groups such as mercury and plutonium, respectively, the database uses the italicized name for data specific to the pure element as well as data for the group in general. For example, non-cancer benchmarks for both elemental mercury and the mercury group are listed under "Mercury and Compounds," the italicized name in the mercury group.

As a final note, the data sources occasionally presented data applicable to the general group names (based on the reported CAS number) using chemical names that were more descriptive than the names used in the database. Although the database typically does not include multiple synonyms for the same compound, some names were judged sufficiently informative to warrant their use in the database. For example, "Mercury (elemental vapor)" provides information about the nature of the mercury at the time of exposure that the database's name, "Mercury and Compounds" does not. For all searches except the Benchmark Summary, the database uses the descriptive name were it applies. The database design does not allow the user to specifically search for data using these more descriptive names; however, these data can be retrieved from searches for data on the corresponding chemical group or on the generic name normally used in the database. Thus, while the user cannot search on "Mercury (elemental vapor)," these data will be retrieved from a search on the "mercury" group or on "Mercury and Compounds."

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Exhibit B-1 indicates the descriptive names used in the database by indenting them under the generic name for which they substitute. For example, the name "Nickel (refinery dust)" is indented under the name "Nickel and Compounds." Thus, the latter is the normal database name for nickel and the nickel group, and the indented name is a variation that may appear in the database output.

EXAMPLE OF LISTING IN EXHIBIT B-1 WITH NOTES IN PARENTHESES									
Chemical Group	Chemical Name	CAS Number	<u>Description</u>						
Nickel			(Name of chemical group)						
	Nickel and Compounds	7440-02-0	(Name normally used for data applicable to						
			nickel or the nickel group)						
	Nickel (refinery dust)		(Alternate name used occasionally where						
			appropriate in the database instead of						
			"Nickel and Compounds." The CAS						
			number, 7440-02-0, does not change)						
	Nickel acetate	373-02-4	(Individual chemicals, with distinct						
	Nickel carbonyl	13463-39-3	CAS numbers, belonging to the nickel						
	-		group)						

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LIST OF CHEMICAL GROUPS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

Chemical Group	Chemical Name	CAS Number*			
Antimony	Antimony and Compounds Antimony (metallic)	7440-36-0			
	Antimony (metanic) Antimony pentafluoride	7783-70-2			
	Antimony pentaridoride Antimony pentoxide	1314-60-9			
	Antimony potassium tartrate	304-61-0			
	Antimony potassium tarrate Antimony tetroxide	1332-81-6			
	Antimony terroxide Antimony trioxide	1309-64-4			
	Antimony trioxide Antimony trisulfide	1345-04-6			
	Antimony distinct	13+3-0+-0			
Arsenic	Arsenic and Compounds Arsenic (inorganic)	7440-38-2			
	Arsenic chloride	7784-34-1			
	Arsenic oxide	1327-53-3			
	Arsenic pentoxide	1303-28-2			
	Arsine	7784-42-1			
Beryllium	Beryllium and Compounds	7440-41-7			
Del ymum	Beryl ore	1302-52-9			
	Beryllium carbonate	66104-24-3			
	Beryllium chloride	7787-47-5			
	Beryllium fluoride	7787-49-7			
	Beryllium hydrogen phosphate	13598-15-7			
	Beryllium nitrate	13597-99-4			
	Beryllium orthophosphate	35089-00-0			
	Beryllium oxide	1304-56-9			
	Beryllium sulfate	13510-49-1			
	Zinc beryllium silicate	39413-47-3			
Cadmium	Cadmium and Compounds	7440-43-9			
	Cadmium oxide	1306-19-0			
	Cadmium stearate	2223-93-0			
Chromium	Chromium and Compounds	7440-47-3			
	Chromium (III) Compounds	16065-83-1			
	Chromium (VI) Compounds	18540-29-9			
	Chromium chloride	10025-73-7			
Cobalt	Cobalt and Compounds	7440-48-4			
	Cobalt acetate	71-48-7			
	Cobalt bromide	7789-43-7			
	Cobalt carbonate	513-79-1			
	Cobalt carbonyl	10210-68-1			
	Cobalt chloride	7646-79-9			
	Cobalt fluoride	10026-17-2			
	Cobalt nitrate	Co Nitrate			

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LIST OF CHEMICAL GROUPS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

Chemical Group Cobalt (cont'd)	<u>Chemical Name</u> Cobalt oxides (mixed) Cobalt phosphate	CAS Number* COBOXIDES 13455-36-2
	Cobalt sulfate	10124-43-3
	Fluomine	62207-76-5
	Tuomme	02207-70-3
Cresol	Cresols (mixed)	1319-77-3
	Cresol, m-	108-39-4
	Cresol, o-	95-48-7
	Cresol, p-	106-44-5
Cyanide	Cyanide and Compounds	57-12-5
Cyamue	Calcium cyanide	592-01-8
	Chlorine cyanide	506-77-4
	Copper cyanide	544-92-3
	Cyanazine	21725-46-2
	Cyanogen	460-19-5
	Cyanogen bromide	506-68-3
	Cyanogen iodide	506-78-5
	Cyanophos	2636-26-2
	Cyanuric fluoride	675-14-9
	Hydrogen cyanide	74-90-8
	Potassium cyanide	151-50-8
	Potassium silver cyanide	506-61-6
	Potassium thiocyanate	333-20-0
	Silver cyanide	506-64-9
	Sodium cyanide	143-33-9
	Thiocyanic acid, 2-(Benzothiazolylthio) methyl ester	21564-17-0
	Zinc cyanide	557-21-1
Dialkylanilines	Diethyl/dimethylaniline, N,N-	Dialks
Diankylammics	Diethylaniline, N,N-	91-66-7
	Dimethylaniline, N,N-	121-69-7
	Difficulty faithfule, 14,14-	121-09-7
DDD/DDE/DDT	DDD	72-54-8
	DDE	72-55-9
	DDT	50-29-3
Dioxin/Furan	Chlorinated dibenzo-p-dioxins (as 2,3,7,8-equivalents)	dioxins
	Chlorinated dibenzofurans (as 2,3,7,8-equivalents)	furans
	Hexachlorodibenzo-p-dioxin, mixture	19408-74-3
	Pentachlorodibenzofuran, 2,3,4,7,8-	57117-31-4
	Tetrachlorodibenzo-p-dioxin, 2,3,7,8-	1746-01-6
	reactionologicenzo-p-dioxiii, 2,3,7,0-	1/70-01-0

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LIST OF CHEMICAL GROUPS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

Chemical Group	Chemical Name	CAS Number*
Glycol ether	Glycol ethers	Glyc Eth
	Diethylene glycol monobutyl ether	112-34-5
	Diethylene glycol monoethyl ether	111-90-0
	Ethylene glycol butyl ether	111-76-2
	Ethylene glycol ethyl ether	110-80-5
	Ethylene glycol ethyl ether acetate	111-15-9
	Ethylene glycol methyl ether	109-86-4
	Ethylene glycol methyl ether acetate	110-49-6
	Propylene glycol monoethyl ether	52125-53-8
	Propylene glycol monomethyl ether	107-98-2
	Propylene glycol, allyl ether	1331-17-5
Lead	Lead and Compounds	7439-92-1
	Lead and compounds (inorganic)	
	Lead acetate	301-04-2
	Lead chloride	7758-95-4
	Lead nitrate	10099-74-8
	Lead subacetate	1335-32-6
	Tetraethyl lead	78-00-2
	Tetramethyl lead	75-74-1
Manganese	Manganese and Compounds	7439-96-5
	Manganese (food)	
	Manganese (water)	
	Manganese acetate	638-38-0
	Manganese chloride	7773-01-5
	Manganese dioxide	1313-13-9
	Manganese oxide	1317-35-7
	Manganese salts and oxides	MNSALTOXIDE
	Manganese sulfate	7785-87-7
	Manganese tricarbonyl	12108-13-3
	methylcyclopentadienyl	
Mercury	Mercury and Compounds	7439-97-6
	Mercury (elemental)	
	Mercury (elemental vapor)	
	Mercury (inorganic)	
	Mercury (metallic)	
	Ethylmercuric phosphate	2440-45-1
	Mercuric acetate	1600-27-7
	Mercuric chloride	7487-94-7
	Mercuric nitrate	10045-94-0
	Mercuric oxide	21908-53-2
	Mercuric sulfide	1134-48-5
	Methoxyethylmercuric acetate	151-38-2
	Methyl mercury	22967-92-6
	•	

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LIST OF CHEMICAL GROUPS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

Chemical Group Mercury (cont'd)	Chemical Name Methylmercuric chloride Methylmercuric dicyanamide Phenylmercuric acetate	<u>CAS Number*</u> 115-09-3 502-39-6 62-38-4
Nickel	Nickel and Compounds Nickel (refinery dust) Nickel acetate Nickel carbonyl Nickel chloride Nickel nitrate Nickel oxide Nickel subsulfide Nickel sulfate	7440-02-0 373-02-4 13463-39-3 7718-54-9 13138-45-9 1313-99-1 12035-72-2 7786-81-4
PCB	Polychlorinated biphenyls Aroclor 1016 Aroclor 1221 Aroclor 1242 Aroclor 1248 Aroclor 1254 Aroclor 1260	1336-36-3 12674-11-2 11104-28-2 53469-21-9 12672-29-6 11097-69-1 11096-82-5
Polycyclic Organic Matter	Polycyclic Organic Matter Polycyclic aromatic hydrocarbons Acenaphthene Anthracene Benzo(a)anthracene Benzo(a)pyrene Benzo(b)fluoranthene Benzo(g,h,i)perylene Benzo(k)fluoranthene Chrysene Dibenz(a,h)anthracene Dimethyl anthracene, 9,10- dimethylbenz(a)anthracene, 7,12- Fluoranthene Fluorene Indeno(1,2,3-cd)pyrene Naphthalene Phenanthrene Pyrene	POM PAHs 83-32-9 120-12-7 56-55-3 50-32-8 205-99-2 191-24-2 207-08-9 218-01-9 53-70-3 781-43-1 57-97-6 206-44-0 86-73-7 193-39-5 91-20-3 85-01-8 129-00-0
Radionuclides	Radionuclides Plutonium and Compounds Plutonium nitrate Plutonium oxide	<i>Radio</i> 7440-07-5 14913-29-2 Pu Oxide

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LIST OF CHEMICAL GROUPS IN THE CUMULATIVE EXPOSURE TOXICITY DATABASE

Chemical Group	<u>Chemical Name</u>	CAS Number*
Radionuclides	Radium	7440-14-4
(cont'd)	Uranium and Compounds	7440-61-1
	Uranium dioxide	1334-57-6
	Uranium hexafluoride	7783-81-5
	Uranium peroxide	19525-15-6
	Uranium tetrachloride	10026-10-5
	Uranium tetrafluoride	10049-14-6
	Uranium, soluble salts	URANSOLS
	Uranyl acetate dihydrate	541-09-3
	Uranyl fluoride	13536-84-0
	Uranyl nitrate hexahydrate	13520-83-7
Selenium	Selenium and Compounds	7782-49-2
	Selenium (dietary)	
	Selenium (elemental)	
	Selenium (elemental dust)	
	Hydrogen selenide	7783-07-5
	Potassium selenate	7790-59-2
	Selenic acid	7783-08-6
	Selenious acid	7783-00-8
	Selenium dioxide	7446-08-4
	Selenium disulfide	7488-56-4
	Selenium oxychloride	7791-23-3
	Selenium sulfide	7446-34-6
	Sodium selenate	13410-01-0
	Sodium selenide	1313-85-5
	Sodium selenite	10102-18-8
Xylene	Xylenes (mixed)	1330-20-7
	Xylene, m-	108-38-3
	Xylene, o-	95-47-6
	Xylene, p-	106-42-3

^{*} Chemicals or chemical groups lacking CAS numbers or for which CAS numbers could not be identified have been assigned unique identifiers in the database.

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Appendix C GLOSSARY OF ACRONYMS

Appendix C

GLOSSARY OF ACRONYMS

112(G) -- EPA Clean Air Act Section 112(g) Technical Background Document.

112(DOC) -- Refers to cancer data found in EPA's Clean Air Act Section 112(g) Technical Background Document and/or EPA's Documentation of Proposed De minimis Emission Rates.

ATSDR -- Agency for Toxic Substances and Disease Registry

ATSDR TOXPROF -- ATSDR's Toxicological Profiles on CD-Rom, 1997.

CAL EPA -- California Environmental Protection Agency

CSF -- Cancer slope factor: The cancer risk per unit of oral exposure. The units of the slope factor are usually expressed as $(mg/kg*day)^{-1}$.

EHS -- EPA's Technical Guidance for Hazards Analysis, Emergency Planning for Extremely Hazardous Substances. This source provides LOC data.

EPA -- U.S. Environmental Protection Agency

HAPfacts -- EPA's Health Effects Notebook for Hazardous Air Pollutants.

HAPS Profiles -- EPA's Hazardous Air Pollutants: Profiles of Non-cancer Toxicity from Inhalation Exposures.

HEAST -- EPA's Health Effects Assessment Summary Tables

IARC - International Agency for Research on Cancer

IRIS -- EPA's Integrated Risk Information System

LOAEL -- Lowest Observed Adverse Effect Level. The lowest exposure dose or concentration at which there is a significant increase in the severity or frequency of an adverse health effect between the exposed population and the control group.

 LC_{50} -- Inhalation exposure concentration that is lethal to 50 percent of the test population.

 LD_{50} -- Oral dose that is lethal to 50 percent of the test population.

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LOC -- Levels of Concern for chemicals on the Superfund Amendments and Reauthorization Act (SARA) Title IV Section 302 list of extremely hazardous substances. LOC is defined as the airborne concentration above which there may be serious permanent health effects from a single acute exposure. EPA bases its estimate of LOC values on one-tenth of the Immediately Dangerous to Life and Health values generated by NIOSH.

MRL -- ATSDR's Minimal Risk Levels. MRLs represent the maximum exposure levels that would not lead to the development of non-cancer health effects in humans, based on acute, subchronic, or chronic exposures.

NOAEL -- No Observed Adverse Effect Level. The highest exposure dose or concentration at which there is no significant increase in the severity or frequency of adverse health effects between the exposed population and the control group.

PAH -- Polycyclic Aromatic Hydrocarbon.

REL -- Reference Exposure Level. Non-cancer benchmarks for inhalation exposures developed by CAL EPA for its Air Toxics "Hot Spots" Program.

RfC -- Reference Concentration. An estimate (with uncertainty spanning perhaps an order of magnitude) of a continuous inhalation exposure level to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious non-cancer effects during a lifetime.

RfD -- Reference Dose. An estimate (with uncertainty spanning perhaps an order of magnitude) of a continuous oral exposure level to the human population (including sensitive subgroups) that is likely to be without an appreciable risk of deleterious non-cancer effects during a lifetime.

Sub-RfC -- An estimate of a subchronic inhalation exposure level to the human population that is likely to be without an appreciable risk of deleterious non-cancer effects.

Sub-RfD -- An estimate of a subchronic oral exposure level to the human population that is likely to be without an appreciable risk of deleterious non-cancer effects.

TEF -- Toxic Equivalency Factor. As used in this manual, a coefficient that compares the cancer potency of a polycyclic aromatic hydrocarbon compound (PAH) to that of the reference PAH, benzo(a)pyrene.

UR -- Unit Risk. The upper bound excess lifetime cancer risk estimated to result from continuous exposure to a compound at a concentration of 1 μ g/L in water or 1 μ g/cum in air.

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WOE -- Weight of evidence for carcinogenicity. The extent to which available biomedical data support the hypothesis that a substance causes cancer in humans. EPA's WOE ranking scale ranges from a high of A to a low of E, and IARC's scale ranges from 1 to 4. Exhibit C-1 provides descriptions of the different WOE categories. Note: WOE categories E (EPA) and 4 (IARC) are rarely used.

	Exhibit C-1								
	DESCRIPTION OF EPA AND IARC WEIGHT OF EVIDENCE CLASSIFICATIONS								
EPA IARC Description of Category									
A	1	Human carcinogen							
В1	2A	Probable human carcinogen limited human evidence							
B2	2A	Probable human carcinogen sufficient evidence in animals and inadequate or no evidence in humans							
С	2B	Possible human carcinogen							
D	D 3 Not classifiable as to human carcinogenicity								
Е	4	Evidence of noncarcinogenicity for humans							

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Appendix D SAMPLE SEARCH OUTPUT

SAMPLE OUTPUT:

CARCINOGENIC RISK-BASED CONCENTRATION BENCHMARKS, CUMULATIVE EXPOSURE OPTION, MEDIUM = WATER

Carcinogenic Risk-Based Concentration Benchmarks

					W		Risk-Based	RBC			Medium/	
Chemical Name	CAS No.	CSF	Unit Risk	UR Units	IARC	EPA	Concentration	Units	Source	Year	Route	Tier
Arsenic (inorganic)	7440-38-2	1.5E+00	5.1E-04	(ug/L)^-1	1	A	1.9E-03	(ug/L)	IRIS	1997	Water	I
Benzene	71-43-2	2.9E-02	9.9E-06	(ug/L)^-1	1	A	1.0E-01	(ug/L)	IRIS	1997	Water	I
Bromodichloromethane	75-27-4	6.2E-02	2.1E-05	(ug/L)^-1	2B	B2	4.7E-02	(ug/L)	IRIS	1997	Water	I
Cadmium and Compounds	7440-43-9			(ug/L)^-1	1	B1			EPA/IARC	1997	Water	
Carbon tetrachloride	56-23-5	1.3E-01	4.5E-05	(ug/L)^-1	2B	B2	2.2E-02	(ug/L)	IRIS	1997	Water	I
Chlorobenzene	108-90-7			(ug/L)^-1		D			EPA/IARC	1997	Water	
Chloroform	67-66-3	6.1E-03	2.1E-06	(ug/L)^-1	2B	B2	4.8E-01	(ug/L)	IRIS	1997	Water	I
Dibromochloromethane	124-48-1	8.4E-02	2.9E-05	(ug/L)^-1	3	C	3.5E-02	(ug/L)	IRIS	1997	Water	I
Ethyl benzene	100-41-4			(ug/L)^-1		D			EPA/IARC	1997	Water	
Ethylene dibromide	106-93-4	8.5E+01	2.9E-02	(ug/L)^-1	2A	B2	3.4E-05	(ug/L)	IRIS	1997	Water	I
Ethylene dichloride	107-06-2	9.1E-02	3.1E-05	(ug/L)^-1	2B	B2	3.2E-02	(ug/L)	IRIS	1997	Water	I
Ethylidene dichloride	75-34-3	5.7E-03	2.0E-06	(ug/L)^-1		C	5.1E-01	(ug/L)	CAL EPA	1996	Water	IIb
Lead and compounds (inorganic)	7439-92-1			(ug/L)^-1	2B	B2			EPA/IARC	1997	Water	
Mercury (elemental vapor)	7439-97-6			(ug/L)^-1		D			EPA/IARC	1997	Water	
Methyl chloride	74-87-3	1.3E-02	4.5E-06	(ug/L)^-1		C	2.2E-01	(ug/L)	HEAST	1997	Water	IIc

Carcinogenic Risk-Based Concentration Benchmarks

Chemical Name	CAS No.	CSF	Unit Risk	UR Units		OE EPA	Risk-Based Concentration	RBC Units	Source	Year	Medium/ Route	Tier
Methyl chloroform	71-55-6			(ug/L)^-1		D			EPA/IARC	1997	Water	
Methylene chloride	75-09-2	7.5E-03	2.6E-06	(ug/L)^-1	2B	В2	3.9E-01	(ug/L)	IRIS	1997	Water	I
Radionuclides	Radio			(ug/L)^-1		A			EPA/IARC	1994	Water	
Radon	14859-67-7			(ug/L)^-1	1				EPA/IARC	1997	Water	
Selenium and Compounds	7782-49-2			(ug/L)^-1		D			EPA/IARC	1997	Water	
Styrene	100-42-5			(ug/L)^-1	2B				EPA/IARC	1997	Water	
Tetrachloroethene	127-18-4	5.1E-02	1.7E-05	(ug/L)^-1	2A	В2-С	5.7E-02	(ug/L)	CAL EPA	1996	Water	IIb
Toluene	108-88-3			(ug/L)^-1	3	D			EPA/IARC	1997	Water	
Trichloroethylene	79-01-6	1.5E-02	5.1E-06	(ug/L)^-1	2A	В2-С	1.9E-01	(ug/L)	CAL EPA	1996	Water	IIb
Vinyl chloride	75-01-4	2.7E-01	9.3E-05	(ug/L)^-1	1	A	1.1E-02	(ug/L)	CAL EPA	1996	Water	IIb
Xylenes (mixed)	1330-20-7			(ug/L)^-1		D			EPA/IARC	1997	Water	

Summary of Sources Hierarchy for Cancer Studies

Exposure Route	Tier	Number Of Chemicals
Oral		
	I	9
	IIb	4
	IIc	1

SAMPLE OUTPUT:

CARCINOGENIC RISK-BASED CONCENTRATION BENCHMARKS, ALL CHEMICALS OPTION, ROUTE = ORAL

Carcinogenic Risk-Based Concentration Benchmarks

a	a.a	607			WO		Risk-Based	RBC	~		Medium/	
Chemical Name	CAS No.	CSF	Unit Risk	UR Units	IARC	EPA	Concentration	Units	Source	Year	Route	Tier
Acephate	30560-19-1	8.7E-03				C	1.1E-04	(mg/kg/day)	IRIS	1997	Oral	I
Acetaldehyde	75-07-0				2B	B2			EPA/IARC	1997		
Acetamide	60-35-5	7.0E-02			2B		1.4E-05	(mg/kg/day)	CAL EPA	1996	Oral	IIb
Acetophenone	98-86-2					D			EPA/IARC	1997		
Acrolein	107-02-8				3	C			EPA/IARC	1997		
Acrylamide	79-06-1	4.5E+00			2A	B2	2.2E-07	(mg/kg/day)	IRIS	1997	Oral	I
Acrylonitrile	107-13-1	5.4E-01			2A	B1	1.9E-06	(mg/kg/day)	IRIS	1997	Oral	I
Alachlor	15972-60-8	8.0E-02				B2	1.2E-05	(mg/kg/day)	HEAST	1997	Oral	IIc
Aldicarb	116-06-3				3	D			EPA/IARC	1997		
Aldrin	309-00-2	1.7E+01			3	B2	5.9E-08	(mg/kg/day)	IRIS	1997	Oral	I
Allyl chloride	107-05-1	2.1E-02			3	C	4.8E-05	(mg/kg/day)	CAL EPA	1996	Oral	IIb
4-aminobiphenyl	92-67-1	2.1E+01			1		4.8E-08	(mg/kg/day)	CAL EPA	1996	Oral	IIb
Aniline	62-53-3	5.7E-03			3	B2	1.8E-04	(mg/kg/day)	IRIS	1997	Oral	I
Anisidine	90-04-0	1.4E-01			2B		7.1E-06	(mg/kg/day)	CAL EPA	1996	Oral	IIb
Anthracene	120-12-7				3	D			EPA/IARC	1997		

Carcinogenic Risk-Based Concentration Benchmarks

					WC		Risk-Based	RBC	_		Medium/	
Chemical Name	CAS No.	CSF	Unit Risk	UR Units	IARC	EPA	Concentration	Units	Source	Year	Route	Tier
Antimony trioxide	1309-64-4				2B	B2			EPA/IARC	1997		
Arsenic (inorganic)	7440-38-2	1.5E+00			1	A	6.7E-07	(mg/kg/day)	IRIS	1997	Oral	I
Arsine	7784-42-1					A			EPA/IARC	1994		
Asbestos	1332-21-4				1	A			EPA/IARC	1997	,	
Atrazine	1912-24-9	2.2E-01			2B	C	4.5E-06	(mg/kg/day)	HEAST	1997	Oral	IIc
Benzene	71-43-2	2.9E-02			1	A	3.4E-05	(mg/kg/day)	IRIS	1997	Oral	I
Benzo(a)anthracene	56-55-3	7.3E-01			2A	B2	1.4E-06	(mg/kg/day)	EPA TEF	1993	Oral	IId
Benzo(a)pyrene	50-32-8	7.3E+00			2A	B2	1.4E-07	(mg/kg/day)	IRIS	1997	Oral	I
Benzo(b)fluoranthene	205-99-2	7.3E-01			2B	B2	1.4E-06	(mg/kg/day)	EPA TEF	1993	Oral	IId
Benzo(g,h,i)perylene	191-24-2					D			EPA/IARC	1997		
Benzo(k)fluoranthene	207-08-9	7.3E-02			2B	B2	1.4E-05	(mg/kg/day)	EPA TEF	1993	Oral	IId
Benzotrichloride	98-07-7	1.3E+01			2B	B2	7.7E-08	(mg/kg/day)	IRIS	1997	Oral	I
Benzyl chloride	100-44-7	1.7E-01			2B	B2	5.9E-06	(mg/kg/day)	IRIS	1997	Oral	I
Beryllium and Compounds	7440-41-7	4.3E+00			1	B2	2.3E-07	(mg/kg/day)	IRIS	1997	Oral	I
Beryllium oxide	1304-56-9	7.0E+00					1.4E-07	(mg/kg/day)	CAL EPA	1996	Oral	IIb

Summary of Sources Hierarchy for Cancer Studies

Exposure Route	Tier	Number Of Chemicals
Oral		
	I	47
	IIa	16
	IIb	28
	IIc	6
	IId	5

SAMPLE OUTPUT:

CHRONIC NON-CARCINOGENIC BENCHMARKS, CUMULATIVE EXPOSURE OPTION, MEDIUM = AIR

Chronic Non-carcinogenic Benchmarks

			Benchmark					Medium/	
Chemical Name	CAS No.	Benchmark	Value	Units	Health Effect Group	Health Effect Descriptor	Tier	Year	Route
Acetaldehyde	75-07-0	RfC	9.0E-03	mg/cu m	Respiratory	Degeneration of olfactory epithelium	I	1997	Air
Acrolein	107-02-8	RfC	2.0E-05	mg/cu m	Respiratory	Squamous metaplasia and neutrophilic infiltration of nasal enithelium	I	1997	Air
Acrylamide	79-06-1	REL	7.0E-04	mg/cu m	unspecified	Unspecified	IIa	1996	Air
Acrylic acid	79-10-7	RfC	1.0E-03	mg/cu m	Respiratory	Degeneration of the nasal olfactory	I	1997	Air
Acrylonitrile	107-13-1	RfC	2.0E-03	mg/cu m	Respiratory	Degeneration and inflammation of nasal	I	1997	Air
Allyl chloride	107-05-1	RfC	1.0E-03	mg/cu m	Neurological	Functional and histological peripheral	I	1997	Air
Aniline	62-53-3	RfC	1.0E-03	mg/cu m	unspecified	Lack of spleen toxicity	I	1997	Air
Arsenic and Compounds	7440-38-2	REL	5.0E-04	mg/cu m	unspecified	Unspecified	IIa	1996	Air
Benzene	71-43-2	REL	7.1E-02	mg/cu m	unspecified	Unspecified	IIa	1996	Air
Benzyl chloride	100-44-7	REL	1.2E-02	mg/cu m	unspecified	Unspecified	IIa	1996	Air
Beryllium and Compounds	7440-41-7	REL	4.8E-06	mg/cu m	unspecified	unspecified	IIa	1996	Air
Bis(2-ethylhexyl)phthalate	117-81-7	REL	7.0E-02	mg/cu m	unspecified	unspecified	IIa	1996	Air
Cadmium and Compounds	7440-43-9	REL	3.5E-03	mg/cu m	unspecified	Unspecified	IIa	1996	Air
Carbon disulfide	75-15-0	RfC	7.0E-01	mg/cu m	Neurological	Peripheral nervous system dysfunction	I	1997	Air
Carbon tetrachloride	56-23-5	REL	2.4E-03	mg/cu m	unspecified	Unspecified	IIa	1996	Air

Chronic Non-carcinogenic Benchmarks

Chemical Name	CAS No.	AS No. Benchmark		Units	Health Effect Group	Health Effect Descriptor	Tier	Year	Medium/ Route
Chlordane	57-74-9	MRL	2.0E-05	mg/cu m	Hepatic	unspecified	IIb	1997	Air
Chlorinated dibenzo-p-dioxins (as 2,3,	dioxins	REL	3.5E-09	mg/cu m	unspecified	unspecified	IIa	1996	Air
Chlorinated dibenzofurans (as 2,3,7,8-	furans	REL	3.5E-09	mg/cu m	unspecified	unspecified	IIa	1996	Air
Chlorobenzene	108-90-7	REL	7.0E-02	mg/cu m	unspecified	Unspecified	IIa	1996	Air
Chloroform	67-66-3	REL	3.5E-02	mg/cu m	unspecified	Unspecified	IIa	1996	Air
Chloroprene	126-99-8	REL	1.0E-03	mg/cu m	unspecified	Unspecified	IIa	1996	Air
Chromium (VI) Compounds	18540-29-9	REL	2.0E-06	mg/cu m	unspecified	Unspecified	IIa	1996	Air
Cresols (mixed)	1319-77-3	REL	1.8E-01	mg/cu m	unspecified	unspecified	IIa	1996	Air
Cumene	98-82-8	RfC	4.0E-01	mg/cu m	Endocrine/Renal	Increased kidney weights in female rats and adrenal weights in male and female rats	I	1997	Air
p-dichlorobenzene	106-46-7	RfC	8.0E-01	mg/cu m	Hepatic	Increased liver weights in P1 males	I	1997	Air
1,3-dichloropropene	542-75-6	RfC	2.0E-02	mg/cu m	Respiratory	Hypertrophy/hyperplasia of the nasal respiratory epithelium	I	1997	Air
Dichlorvos	62-73-7	RfC	5.0E-04	mg/cu m	Neurological	Decreased brain cholinesterase activity	I	1997	Air
Dimethyl formamide	68-12-2	RfC	3.0E-02	mg/cu m	Gastrointestinal/Hepatic	Digestive disturbances and minimal hepatic changes suggestive of liver abnormalities	I	1997	Air
1,4-dioxane	123-91-1	REL	4.0E-01	mg/cu m	unspecified	unspecified	IIa	1996	Air
Epichlorohydrin	106-89-8	RfC	1.0E-03	mg/cu m	Respiratory	Changes in the nasal turbinates	I	1997	Air

Summary of Chronic Non-carcinogenic Tiers

Exposure Route	Tier	NumberOfChemicals
Inhalation		
	I	32
	IIa	47
	IIb	2

SAMPLE OUTPUT:

ACUTE NON-CARCINOGENIC RISK-BASED CONCENTRATION BENCHMARKS, ALL CHEMICALS OPTION, ROUTE = ORAL AND INHALATION

Acute Non-carcinogenic Benchmarks

				Benchmark						Route/
Chemical Name	CAS No.	Species	Benchmark	Value	Units	Health Effect Grouping	Citation	Tier	Year	Medium
Acetaldehyde	75-07-0	rat	LC50	3.6E+04	mg/cu m	Death	Skog, 1950	Ш	1993	Inhalation
Acetonitrile	75-05-8	rat	LC50	1.3E+04	mg/cu m	Death	Verschueren, Handbook Environ. Data	Ш	1993	Inhalation
Acrolein	107-02-8		LOC	1.2E-03	mg/cu m	unspecified		IIa	1994	Inhalation
Acrolein	107-02-8	rat	LD50	4.6E+01	mg/kg/day	Death	Smyth et al. 1951	III	1990	Oral
Acrylamide	79-06-1		LOC	1.1E-01	mg/cu m	unspecified		IIa	1987	Inhalation
Acrylic acid	79-10-7		RfD	5.0E-01	mg/kg/day	Developmental		I	1997	Oral
Acrylic acid	79-10-7	rat	LC50	3.5E+03	mg/cu m	Death	Majka et al., 1979	Ш	1993	Inhalation
Acrylonitrile	107-13-1		MRL	1.0E-01	mg/kg/day	Developmental		II	1997	Oral
Acrylonitrile	107-13-1		LOC	1.1E-01	mg/cu m	unspecified		IIa	1987	Inhalation
Aldicarb	116-06-3		LOC	3.0E-04	mg/cu m	unspecified		IIa	1987	Inhalation
Aldrin	309-00-2		MRL	2.0E-03	mg/kg/day	Developmental		II	1997	Oral
Aldrin	309-00-2		LOC	1.0E-02	mg/cu m	unspecified		IIa	1987	Inhalation
Aniline	62-53-3		LOC	3.8E-02	mg/cu m	unspecified		IIa	1987	Inhalation
Antimony pentafluoride	7783-70-2		LOC	2.7E-03	mg/cu m	unspecified		IIa	1994	Inhalation
Aroclor 1016	12674-11-2		RfD	7.0E-05	mg/kg/day	Developmental		I	1997	Oral
Aroclor 1221	11104-28-2	mink	LD50	7.5E+02	mg/kg/day	Death	Aulerich and Ringer 1977	Ш	1995	Oral
Aroclor 1242	53469-21-9	rat	LD50	4.3E+03	mg/kg/day	Death	Bruckner et al. 1973	III	1995	Oral

Acute Non-carcinogenic Benchmarks

Chemical Name	CAS No.	Species	Benchmark	Benchmark Value	units	Health Effect Grouping	Citation	Tier	Year	Route/ Medium
Aroclor 1254	11097-69-1	rat	LD50	1.0E+03	mg/kg/day	Death	Garthoff et al. 1981	III	1995	Oral
Aroclor 1260	11096-82-5	rat	LD50	1.3E+03	mg/kg/day	Death	Linder et al. 1974	III	1995	Oral
Arsenic and Compounds	7440-38-2	rat	LD50	1.5E+01	mg As/kg/day	Death	Harrisson et al. 1958	III	1993	Oral
Arsenic chloride	7784-34-1		LOC	1.0E-02	mg/cu m	unspecified		IIa	1987	Inhalation
Arsenic oxide	1327-53-3		LOC	1.4E-03	mg/cu m	unspecified		IIa	1994	Inhalation
Arsenic pentoxide	1303-28-2		LOC	8.0E-03	mg/cu m	unspecified		IIa	1994	Inhalation
Arsine	7784-42-1		LOC	1.9E-03	mg/cu m	unspecified		IIa	1994	Inhalation
Azinphos-methyl	86-50-0		LOC	7.0E-04	mg/cu m	unspecified		IIa	1987	Inhalation
Benzene	71-43-2	rat	LD50	9.3E+02	mg/kg/day	Death	Cornish and Ryan 1965	III	1995	Oral
Benzene	71-43-2		MRL	1.6E-01	mg/cu m	Immunological		IIb	1997	Inhalation
Benzotrichloride	98-07-7		LOC	7.0E-04	mg/cu m	unspecified		IIa	1994	Inhalation
Benzyl chloride	100-44-7		LOC	5.2E-03	mg/cu m	unspecified		IIa	1994	Inhalation
Beryllium chloride	7787-47-5	rat	LD50	2.0E+02	mg Be/kg/day	Death	Kimmerle 1966	III	1993	Oral
Beryllium fluoride	7787-49-7	rat	LD50	1.9E+01	mg Be/kg/day	Death	Venugopal and Luckey 1977	III	1993	Oral
Beryllium orthophosphate	35089-00-0	rat	LC50	8.6E-01	mg Be/cu m	Death	Venugopal and Luckey 1977	III	1993	Inhalation
Beryllium sulfate	13510-49-1	rat	LD50	1.2E+02	mg Be/kg/day	Death	Lanchow 1978	III	1993	Oral
Beryllium sulfate	13510-49-1	rat	LC50	1.5E-01	mg Be/cu m	Death	Venugopal and Luckey 1977	III	1993	Inhalation

Summary of Acute Non-carcinogenic Tiers

Exposure Route	Tier	Number Of Chemicals	
Inhalation			
	I	3	
	IIa	90	
	IIb	17	
	III	27	
Oral			
	I	7	
	II	39	
	III	54	

SAMPLE OUTPUT:

TOXICITY BENCHMARK SUMMARY, CUMULATIVE EXPOSURE OPTION, MEDIUM = AIR

Summary of Toxicity Benchmarks - Air Exposure

Chemical Name	CAS Number	Risk-Based Conc.*	IARC WOE	EPA WOE	Carcin Tier	Chronic Benchmark*	Chronic BM Type	Chronic Tier	Acute Benchmark*	Acute BM Type	Acute Tier
Acetaldehyde	75-07-0	4.5E-01	2B	B2	I	9.0E-03	RfC	I	3.6E+04	LC50	III
Acetamide	60-35-5	5.0E-02	2B		IIc						
Acetonitrile	75-05-8								1.3E+04	LC50	III
Acetophenone	98-86-2			D							
Acrolein	107-02-8		3	C		2.0E-05	RfC	I	1.2E-03	LOC	IIa
Acrylamide	79-06-1	7.7E-04	2A	B2	I	7.0E-04	REL	IIa	1.1E-01	LOC	IIa
Acrylic acid	79-10-7					1.0E-03	RfC	I	3.5E+03	LC50	Ш
Acrylonitrile	107-13-1	1.5E-02	2A	B1	I	2.0E-03	RfC	I	1.1E-01	LOC	IIa
Allyl chloride	107-05-1	1.7E-01	3	C	IIc	1.0E-03	RfC	I			
Aniline	62-53-3	6.1E-01	3	B2	IIb	1.0E-03	RfC	I	3.8E-02	LOC	IIa
Anisidine	90-04-0	2.5E-02	2B		IIc						
Arsenic and Compounds	7440-38-2	2.3E-04	1	A	I	5.0E-04	REL	IIa			
Benzene	71-43-2	1.2E-01	1	A	I	7.1E-02	REL	IIa	1.6E-01	MRL	IIb
Benzotrichloride	98-07-7	2.7E-04	2B	B2	IIb				7.0E-04	LOC	IIa
Benzyl chloride	100-44-7	2.1E-02	2B	B2	IIb	1.2E-02	REL	IIa	5.2E-03	LOC	IIa

^{*} Inhalation carcinogenic risk-based concentrations are in ug/cu m, and non-carcinogenic benchmarks are in mg/cu m.

Summary of Toxicity Benchmarks - Air Exposure

Chemical Name	CAS Number	Risk-Based Conc.*	IARC WOE	EPA WOE	Carcin Tier	Chronic Benchmark*	Chronic BM Type	Chronic Tier	Acute Benchmark*	Acute BM Type	Acute Tier
Beryllium and Compounds	7440-41-7	4.2E-04	1	B2	I	4.8E-06	REL	IIa			
Biphenyl	92-52-4			D							
Bis(2-ethylhexyl)phthalate	117-81-7	2.5E-01	2B	B2	IIb	7.0E-02	REL	IIa			
Bis(chloromethyl)ether	542-88-1	1.6E-05	1	A	I				2.5E-04	LOC	IIa
Bromoform	75-25-2	9.1E-01	3	B2	I						
1,3-butadiene	106-99-0	3.6E-03	2A	B2	I				4.4E+00	LOC	IIa
Cadmium and Compounds	7440-43-9	5.6E-04	1	B1	I	3.5E-03	REL	IIa			
Captan	133-06-2	1.5E+00	3	B2	IIc						
Carbon disulfide	75-15-0					7.0E-01	RfC	I	1.6E-01	LOC	IIa
Carbon tetrachloride	56-23-5	6.7E-02	2B	B2	I	2.4E-03	REL	IIa	1.3E+00	MRL	IIb
Chlordane	57-74-9	2.7E-03	2B	B2	I	2.0E-05	MRL	IIb	5.0E-02	LOC	IIa
Chlorinated dibenzo-p-dioxins (as 2,3,7,8-	dioxins			B2		3.5E-09	REL	IIa			
Chlorinated dibenzofurans (as 2,3,7,8-equ	furans			B2		3.5E-09	REL	IIa			
Chloroacetic acid	79-11-8								1.8E-03	LOC	IIa
Chlorobenzene	108-90-7			D		7.0E-02	REL	IIa	8.7E+03	LC50	III

^{*} Inhalation carcinogenic risk-based concentrations are in ug/cu m, and non-carcinogenic benchmarks are in mg/cu m.

Tier Summary - Air Exposure

Exposure Route	Type	Tier	Number of Chemicals	
Inhalation				
	Cancer			
		I	31	
		IIa	7	
		IIb	9	
		IIc	18	
		IId	1	
	Chronic NC			
		I	31	
		IIa	47	
		IIb	2	
	Acute NC			
		I	3	
		IIa	41	
		IIb	16	
		Ш	18	

SAMPLE OUTPUT:

SEARCH BY CHEMICAL: ORAL LOAELS, NOAELS, AND LD50S FOR ACENAPHTHENE, BENZENE, AND VINYL CHLORIDE

NOAELs, LOAELs, & LD50s

Chemical Name	CAS Number	Exposure Type	Species	Sex	Type of Benchmark	Benchmark Value	Units	Health Effect Grouping	Health Effect Descriptor	Citation
Acenaphthene	83-32-9	subchronic	mouse		LOAEL	1.8E+02	mg/kg/day	Hepatic	Increased relative liver weight	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse	f	LOAEL	7.0E+02	mg/kg/day	Reproductive	Decreased ovary weights correlated with increased incidence and degree of inactivity of the ovary and uterus	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse	f	NOAEL	3.5E+02	mg/kg/day	Reproductive	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Muscular/Skeletal	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Respiratory	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse	m	NOAEL	7.0E+02	mg/kg/day	Reproductive	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Renal	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Neurological	unspecified	EPA 1989e
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Immunological	unspecified	EPA 1989c

NOAELs, LOAELs, & LD50s

Chemical Name	CAS Number	Exposure Type	Species	Sex	Type of Benchmark	Benchmark Value	Units	Health Effect Grouping	Health Effect Descriptor	Citation
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Body Weight	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Gastrointestinal	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Ocular	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Endocrine	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Dermal	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Cardiovascular	unspecified	EPA 1989c
Acenaphthene	83-32-9	subchronic	mouse		NOAEL	7.0E+02	mg/kg/day	Hematological	unspecified	EPA 1989c
Benzene	71-43-2	acute	rat	m	LD50	9.3E+02	mg/kg/day	Death	Unspecified	Cornish and Ryan 1965
Benzene	71-43-2	acute	rat	m	LD50	5.6E+03	mg/kg/day	Death	Unspecified	Wolf et al. 1956

SAMPLE OUTPUT:

SEARCH BY CHEMICAL: CHRONIC EPA RFDS FOR MERCURY CHEMICAL GROUP

Reviewed Benchmarks - Oral

Chemical Name	CAS No.	Exposure Type	Benchmark	EPA Value* WOE	Health Effect Grouping	Health Effect Descriptor	Data Source	Year
Mercuric chloride	7487-94-7	chronic	RfD	3.0E-04	Immunological	Autoimmune effects	IRIS	1997
Methyl mercury	22967-92-6	chronic	RfD	1.0E-04	Developmental	Developmental neurologic abnormalities in human in	IRIS	1997
Phenylmercuric acetate	62-38-4	chronic	RfD	8.0E-05	Renal	Renal damage	IRIS	1997

SAMPLE OUTPUT:

SEARCH BY HEALTH EFFECT: CHRONIC RFDS AND RFCS RELATED TO CARDIOVASCULAR OR RESPIRATORY HEALTH EFFECTS

Non-carcinogenic Health Effect-Specific Data

Chemical Name	CAS No.	Exp. Route	Exp. Type	Bench- mark	Value	Units	Health Effect Group	Health Effect Descriptor	Data Source	Citation
Acetaldehyde	75-07-0	inhalation	chronic	RfC	9.0E-03	mg/cu m	Respiratory	Degeneration of olfactory epith	IRIS	
Acrolein	107-02-8	inhalation	chronic	RfC	2.0E-05	mg/cu m	Respiratory	Squamous metaplasia and neutr	IRIS	
Acrylic acid	79-10-7	inhalation	chronic	RfC	1.0E-03	mg/cu m	Respiratory	Degeneration of the nasal olfac	IRIS	
Acrylonitrile	107-13-1	inhalation	chronic	RfC	2.0E-03	mg/cu m	Respiratory	Degeneration and inflammatio	IRIS	
Antimony trioxide	1309-64-4	inhalation	chronic	RfC	2.0E-04	mg/cu m	Respiratory	Pulmonary toxicity, chronic int	IRIS	
Arsenic (inorganic)	7440-38-2	oral	chronic	RfD	3.0E-04	mg/kg/day	Cardiovascular/Dermal/He	Hyperpigmentation, keratosis a	IRIS	
Chloroacetic acid	79-11-8	oral	chronic	RfD	2.0E-03	mg/kg/day	Cardiovascular	Heart - Myocarditis	HEAST T1	
Chloroprene	126-99-8	inhalation	chronic	RfC	7.0E-03	mg/cu m	Respiratory	Olfactory epithelium - Degener	HEAST T1	
p-cresol	106-44-5	oral	chronic	RfD	5.0E-03	mg/kg/day	Neurological/Respiratory	Central nervous system - Hypo	HEAST T1	
1,3-dichloropropene	542-75-6	inhalation	chronic	RfC	2.0E-02	mg/cu m	Respiratory	Hypertrophy/hyperplasia of the	IRIS	
Epichlorohydrin	106-89-8	inhalation	chronic	RfC	1.0E-03	mg/cu m	Respiratory	Changes in the nasal turbinates	IRIS	
1,2-epoxybutane	106-88-7	inhalation	chronic	RfC	2.0E-02	mg/cu m	Respiratory	Degenerative lesions of the nas	IRIS	
Hexachlorocyclopentadiene	77-47-4	inhalation	chronic	RfC	7.0E-05	mg/cu m	Respiratory	Nasal cavity - Aquamous meta	HEAST T1	
Hydrochloric acid	7647-01-0	inhalation	chronic	RfC	2.0E-02	mg/cu m	Respiratory	Hyperplasia of nasal mucosa, l	IRIS	
Methyl bromide	74-83-9	inhalation	chronic	RfC	5.0E-03	mg/cu m	Respiratory	Degenerative and proliferative	IRIS	

Non-carcinogenic Health Effect-Specific Data

Chemical Name	CAS No.	Exp. Route	Exp. Type	Bench- mark	Value	Units	Health Effect Group	Health Effect Descriptor	Data Source	Citation
Methylene diphenyl diisocya	101-68-8	inhalation	chronic	RfC	2.0E-05	mg/cu m	Respiratory	Hyperplasia of the olfactory ep	IRIS	
Phthalic anhydride	85-44-9	inhalation	chronic	RfC	1.2E-01	mg/cu m	Respiratory	Nose - Rhinitis; Lungs - Bronc	HEAST T1	
Phthalic anhydride	85-44-9	oral	chronic	RfD	2.0E+00	mg/kg/day	Renal/Respiratory	Lung and kidney histopatholog	IRIS	
Propylene oxide	75-56-9	inhalation	chronic	RfC	3.0E-02	mg/cu m	Respiratory	Nest-like folds of the nasal resp	IRIS	
2,4/2,6-toluene diisocyanate	26471-62-5	inhalation	chronic	RfC	7.0E-05	mg/cu m	Respiratory	Chronic lung-function decline	IRIS	
Vinyl acetate	108-05-4	inhalation	chronic	RfC	2.0E-01	mg/cu m	Respiratory	Nasal epithelial lesions	IRIS	

Appendix E

LIST OF DATABASE PROGRAMMING COMPONENTS ASSOCIATED WITH EACH SEARCH

CARCINOGENIC RISK-BASED CONCENTRATION BENCHMARK SEARCH					
CumExp/AllChems - Cancer Report Export					
CreateOral/InhalCancerHealthTable CreateOralCancerHealthTable - AllChems CreateTierSummaryTable CreateTierSummaryTable2 CreateWaterCancerHealthTable					
globalVariables					
InhalTier1b InhalTier2a InhalTier2a InhalTier2a - oral/inhal InhalTier2b InhalTier2b - oral/inhal InhalTier2c InhalTier2c InhalTier2c - oral/inhal OralTier1a OralTier1a - oral/inhal OralTier1b OralTier1b - oral/inhal OralTier2a OralTier2a OralTier2b - oral/inhal OralTier2c OralTier2c - oral/inhal OralTier2c OralTier2c - oral/inhal OralTier2c OralTier2c - oral/inhal					

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CHRONIC NON-CARCINOGENIC	C HEALTH EFFECT BENCHMARK SEARCH
Forms	
CumExp/AllChems - NCchronic NCChronicSources	NCChronicSources - AllChems Report Export
Macros	
mcrNCChronicAir mcrNCChronicAirWaterFood mcrNCChronicFood mcrNCChronicInhal - AllChems	mcrNCChronicInhal/Oral - AllChems mcrNCChronicOral - AllChems mcrNCChronicWater
Modules	
globalVariables	
Queries	
DelNCChronicSources DelNCChronicTierSummary DeltbIINCChronic NCChronicATSDR NCChronicCALEPA NCChronicFood NCCChronicInhal NCChronicInhal - AllChems NCChronicInhalAir NCChronicInhalATSDR NCChronicInhalATSDR NCChronicInhalCALEPA NCChronicInhalCALEPA NCChronicInhalCALEPA - AllChems NCChronicInhalCALEPA - AllChems NCChronicInhalIRIS	NCChronicInhalIRIS - AllChems NCChronicInhalTier1 NCChronicInhalTier2 NCChronicInhalTier3 NCChronicInhalTier4 NCChronicIris NCChronicOral NCChronicOral - AllChems NCChronicOralTier1 NCChronicOralTier2 NCChronicOralTier3 NCChronicOralTier4 NCChronicOralTier4 NCChronicOralTier4
Reports	
NCHealthEffects	rptNCChronicTiers
Tables	
_Gen_Info _Noncancer NCChronicSources	NCChronicTierSummary tblINCChronic

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ACUTE NON-CARCINOGENIC	HEALTH EFFECT BENCHMARK SEARCH
Forms	
CumExp/AllChems - NCAcute NCAcuteSources	NCAcuteSources - AllChems Report Export
Macros	
mcrNCAcuteAir mcrNCAcuteAirWaterFood mcrNCAcuteFood mcrNCAcuteInhal - AllChems mcrNCAcuteInhal/Oral - AllChems	mcrNCAcuteOral - AllChems mcrNCAcuteWater NCAcuteSources NCAcuteSources2
Modules	
globalVariables	
Queries	
DelNCAcute DelNCAcuteSourcesReport DelNCAcuteTierSummary NCAcuteAir NCAcuteFood NCAcuteInhal NCAcuteInhal - AllChems NCAcuteInhalIRIS NCAcuteInhalLC50 NCAcuteInhalLC50first NCAcuteInhalLOC NCAcuteInhalLOC NCAcuteInhalLOC2 NCAcuteInhalMRL Reports	NCAcuteInhalTier1 NCAcuteInhalTier2 NCAcuteInhalTier3 NCAcuteInhalTier4 NCAcuteOral - AllChems NCAcuteOralIRIS NCAcuteOralLD50 NCAcuteOralLD50first NCAcuteOralMRL NCAcuteOralTier1 NCAcuteOralTier1 NCAcuteOralTier3 NCAcuteWater
rptNCAcute	rptNCAcuteTiers
Tables	
_Gen_Info _Noncancer NCAcute	NCAcuteSourcesReport NCAcuteTierSummary

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SUMMARY O	F TOXICITY BENCHMARKS
Forms	
CumExp/AllChems - Summary frmSummaryInfo	frmSummaryInfo - AllChems Report Export
Macros	
Air Tier	mcrInhal/OralSummary - AllChems
CreateCancerSourcesTable	mcrInhalSummary - AllChems
CreateInhalCancerSources	mcrOralSummary - AllChems
FoodTier	mcrWaterSummary
mcrAirSummary	NCAcuteSources
mcrAirWaterFoodSummary	NCAcuteSources2
mcrFoodSummary	WaterTier
Modules	
globalVariables	
Queries	
AirSumAcuTier1	NCAcuteInhalLOC2
AirSumAcuTier2	NCAcuteInhalMRL
AirSumAcuTier3	NCAcuteOral - AllChems
AirSumAcuTier4	NCAcuteOralIRIS
AirSumCanTier1a	NCAcuteOralLD50
AirSumCanTier1b	NCAcuteOralLD50first
AirSumCanTier2a	NCAcuteOralMRL
AirSumCanTier2b	NCAcuteWater
AirSumCanTier2c	NCChronicATSDR
AirSumChrTier1	NCChronicCALEPA
AirSumChrTier2	NCChronicFood
AirSumChrTier3	NCCChronicInhal
AirSumChrTier4	NCChronicInhalATSDR
Cancer112(DOC)Inhal	NCChornicInhalATSDR - AllChems
Cancer112(DOC)Oral	NCChronicInhalCALEPA
CancerCALEPAInhal	NCChronicInhalCALEPA - AllChems
CancerCALEPAOral	NCChronicInhalIRIS
CancerHEASTInhal	NCChronicInhalIRIS - AllChems
CancerHEASTOral	NCChronicIris
CancerIRIS	NCChronicOral
CancerIRISInhal	NCChronicOral - AllChems
CancerIRISOral	NCChronicWater
CancerTEF	qryAirSummary
CancerWOEInhal	qryCancerAir
CancerWOEInhala	qryCancerAir - AllChems
CancerWOEOral	qryCancerAir2
DelAirTier	qryCancerAir2 - AllChems
DeleteCancerAir	qryCancerFood
DeleteCancerFood	qryCancerOral - AllChems
DeleteCancerSources	qryCancerWater
NCAcuteInhalLOC	

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SUMMARY OF TOXICITY BENCHMARKS (continued)

_			
()11	eries	(conti	med)

DeleteCancerWaterqryFoodSummaryDeletetblAirSummaryqryNCAcuteAirSummaryDelFoodTierqryNCAcuteAirSummary1DelNCAcuteqryNCAcuteFoodSummaryDelNCAcuteSourcesReportqryNCAcuteFoodSummarya

DelNCChronicSources qryNCAcuteInhalSummary - AllChems
DeltblFoodSummary qryNCAcuteInhalSummary - AllChems
DeltblINCChronic qryNCAcuteOralSummary - AllChems
DeltblWaterSummary qryNCAcuteOralSummary - AllChems

DelWaterTier qryNCAcuteWaterSummary
FoodSumAcuTier1 qryNCAcuteWaterSummarya
FoodSumAcuTier2 qryNCChronicAirSummary
FoodSumAcuTier3 qryNCChronicFoodSummary
FoodSumCanTier1a qryNCChronicWaterSummary

qryWaterSummary FoodSumCanTier1b FoodSumCanTier2a WaterSumAcuTier1 FoodSumCanTier2b WaterSumAcuTier2 FoodSumCanTier2c WaterSumAcuTier3 FoodSumChrTier1 WaterSumCanTier1a FoodSumChrTier3 WaterSumCanTier1b FoodSumChrTier4 WaterSumCanTier2a NCAcuteAir2Sum WaterSumCanTier2b NCAcuteAir2Sum - AllChems WaterSumCanTier2c **NCAcuteFood** WaterSumChrTier1 WaterSumChrTier3 **NCAcuteInhalIRIS**

NCAcuteInhalLC50first

NCAcuteInhalLC50

Reports

AirSummary InhalTierReport - AllChems
AirTierReport Oral Summary - AllChems
FoodSummary OralTierReport - AllChems
FoodTierReport WaterSummaryTier
InhalSummary - AllChems WaterTierReport

Tables

CancerSources

_Cancer FoodSummaryTier

_Gen_Info NCAcute

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WaterSumChrTier4

WaterSummaryTier

SEARCH BY CHEMICAL						
Forms						
ExpRoute2 GroupChem IndividualChem IndividualChem - CAS InfoType Name/CAS Next NOAELInhal	NOAELOral NoSelection Report Export RevBenchesInhal RevBenchesOral SearchByChem TryAgain - ChemSearch					
Modules						
SelChemMod						
Queries						
ChemGroups						
Reports						
NOAELInhalReport NOAELInhalReport2 NOAELInhalReport3 NOAELOralReport NOAELOralReport2 Tables	NOAELOralReport3 QualInhalReport QualOralReport RevBenchInhalReport RevBenchOralReport					
Cancer	NOAELOralRpt					
Cancer Gen_Info Inhal LOAELs, NOAELs, & LC50s Noncancer Oral LOAELs, NOAELs, & LD50s Qualitative_Health_Effects NOAELInhalRpt	Quallnhal QualOral SelectedChems SelectedGrps SellnhalChemsRpt SelOralChemsRpt					

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SEARCH BY HEALTH EFFECT					
Forms					
ErrorNoDate - HealthEffectSearch	OralData				
ExpRoute	OralInhalData				
HealthEffects	PleaseWait				
InhalData	Report Export				
Next					
Modules					
modNCHealthEffects					
Reports					
NCHealthEffectGrps	NCHealthEffectGrps2				
Tables					
_Gen_Info	_Oral LOAELs, NOAELs, & LD50s				
Inhal LOAELs, NOAELs, & LC50s	NCHealthEffects				
Noncancer	NCHealthEffectsReport				

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SYNONYM GUIDE		
Forms		
SynForm		
Tables		
_Synonyms	SynOutput	

DATABASE COMPONENTS NOT LINKED TO INDIVIDUAL SEARCHES		
Forms		
AllReports Help Help - CancerHierarchy Help - Exporting to Excel Help - Hierarchy Help - NCAcuteHierarchy	Help - NCChronicHierarchy Help - RBC HelpAirWaterFood HelpGroup/IndivChem HelpSynonymGuide	
Macros		
AutoExec		
Tables		
_Data Sources		

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Appendix F

A COMPARISON OF THE CUMULATIVE EXPOSURE TOXICITY DATABASE AND THE CALDWELL ET AL. DATABASE

APPENDIX F

A COMPARISON OF THE CUMULATIVE EXPOSURE TOXICITY DATABASE AND THE CALDWELL ET AL. DATABASE

While the Cumulative Exposure Toxicity Database (CETDB) has wide-ranging applications, it was designed primarily to assist in future analyses of the results from EPA's Cumulative Exposure Study. Previous analysis of the preliminary results of the air portion of the Cumulative Exposure Study utilized a different database of toxicological data developed by EPA's Office of Air Quality Planning and Standards and described in the following reference: Caldwell, Jane C., Tracey J. Woodruff, Rachel Morello-Frosch, and Daniel A. Axelrad, "Application of Health Information to Hazardous Air Pollutants Modeled in EPA's Cumulative Exposure Project," *Toxicology and Industrial Health*, vol. 14, p. 429-54, 1998.

Because the Caldwell et al. database is used to analyze compounds in the air component of the Cumulative Exposure Study, it focuses on toxicity data for the inhalation route of exposure. The CETDB and the Caldwell database share much of the same toxicity data, and certain features of the CETDB (e.g., the data hierarchies) are based on the Caldwell database. However, the two databases are distinctly different in several key ways and are not interchangeable. In order to alleviate potential confusion, we enumerate here the key differences between the CETDB and the Caldwell et al. database.

- Chemicals Included. The CETDB includes data for 344 individual chemicals or chemical groups, approximately half of which were analyzed in either the air, food, or water segments of EPA's Cumulative Exposure Study. The Caldwell et al. database includes toxicity data for 148 hazardous air pollutants (HAPs) analyzed in the air portion of the Cumulative Exposure Study.
- **Data Types.** The CETDB includes some inhalation toxicity data not included in the Caldwell et al. database, specifically LOAELs, NOAELs, and LC₅₀s. The CETDB also includes toxicity measures related to the oral route of exposure (e.g., RfDs, CSFs, and LD₅₀s) that are not included in the Caldwell database.
- **Data Sources.** The CETDB includes data from sources that are not included in the Caldwell database, such as the Agency for Toxic Substances and Disease Registry's (ATSDR) *Toxicological Profiles*, EPA's *Hazardous Air Pollutants: Profiles of Non-cancer Toxicity from Inhalation Exposures*, and EPA's *Health Effects Notebook for Hazardous*

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Air Pollutants. The Caldwell database includes some specific EPA references for data on individual compounds, such as methyl tert-butyl ether, that are not included in the CETDB.

- **Benchmark Oral Data Hierarchies.** Because the Caldwell database focuses on exposure to hazardous air pollutants via inhalation, it does not specify hierarchies for types and sources of toxicity data related to oral exposure. The CETDB has developed hierarchies for its oral data sources that are based upon the inhalation hierarchies in the Caldwell database.
- Cancer Benchmark Inhalation Data Hierarchy. The Caldwell cancer hierarchy differs from that of the CETDB in four major ways:
 - (1) Caldwell includes cancer potency estimates derived from data used to support the derivation of ED_{10} values (effective dose for 10 percent of the population) for Superfund, and the CETDB does not;
 - (2) Caldwell uses EPA oral data analyzed for the Clean Air Act Section 112 technical support documents to derive URs if no UR is available. The CETDB uses IRIS oral data to derive URs if no UR is available;
 - (3) Caldwell assigns a default cancer potency based on the potency of methylene chloride when no other values are available for a compound. The CETDB does not assign a default value in this situation. It presents the WOE if available; otherwise, the compound is not included in the output table;
 - (4) Caldwell does not include a tier for HEAST values. The CETDB does include HEAST in its hierarchy; and
- Non-Cancer Chronic Benchmark Inhalation Data Hierarchy. The Caldwell hierarchy includes provisional EPA inhalation RfCs, while the CETDB does not.
- Non-Cancer Acute Benchmark Inhalation Data Hierarchy. The Caldwell hierarchy includes LOCs/1000 and EPA RfCs for short-term exposure. The CETDB hierarchy includes those benchmarks plus ATSDR acute MRLs and LC₅₀ values.

For further information on the respective data hierarchies, please consult Chapter 2 of the CETDB User's Manual and the Caldwell et al. paper referenced above.

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